4th International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal
July 6-9, 2021

Book of Abstracts

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Gil Alberto Batista Gonçalves
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(4th ICNMSME-2021)

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.

The Organizing Committee ICNMSME2021

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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)

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Conference Web

http://icnmsme2021.web.ua.pt/

ICNMSME2021 program

July 6, 2021 (Tuesday)

Workshop on Low-dimensional materials: experiment, theory, application (WLDM-2021) **University of Aveiro, Portugal, July 6, 2021 (*online*)** **Auditorium 1**	
9:00-9:15	**WELCOME ADDRESS** **Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, Dr. Igor Bdikin**
9:15-10:15	CHAIR: Prof. Dr. Duncan Paul Fagg **The growth- and coalescence behaviour of graphene: Insights from In-situ scanning electron microcopy** **Prof. Dr. Marc Georg Willinger** *ETH Zurich, Department of Materials, Scientific Center for Optical and Electron Microscopy, Zurich, Schweiz*
10:15–10:45	**Coffee break / Open discussions**
10:45–11:15	**2D- Photocatalyst: 6, 13- Pentacenequinone (PQ) for Future** **Prof. Dr. Vikram Uttam Pandit** *Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India*
11:15–12:00	CHAIR: Prof. Dr. Duncan Paul Fagg **Modeling of Low-dimensional & 2D-materials** **Prof. Dr. Vladimir Bystrov** *Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*
12:00–12:30	**Two Dimensional Zinc Oxide (2D-ZnO) Nanostructures for MB Dye Degradation** **VIVEKANAND JAWALE** *Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India*

12:30–14:00	**Lunch break**
14:00–14:45	CHAIR: Dr. Gonzalo Guillermo Otero **Graphene-based nanocomposites with high-performance for health and environmental applications** **Dr. Gil Gonçalves** *TEMA-NRD, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*
14:45–15:15	**Free Vibration Analysis of rotating Single Walled Carbon Nanotubes Resting in Elastic Medium** **Prof. Dr. Abdelkadir Belhadj** *DC Engineering & Project Management, Sonatrach, Algiers, Algeria; Computational Mechanics Laboratory, Faculty of Technology, University of Tlemcen, Tlemcen, Algeria*
15:15–15:45	**Low-dimensional effects in Atomic Force Microscopy (AFM)** **Dr. Igor Bdikin** *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal*
15:45–16:00	**Final discussions and comments**

July 7, 2021(Wednesday)

4th International Conference on Nanomaterials Science and Mechanical Engineering (4th ICNMSME-2021) (*online*)	
9:00-9:30	**Auditorium 1** **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)
9:30-10:20	Session: **New Energy Materials** CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, Dr. Gil Gonçalves ***Plenary Lecture*** Prof. Dr. Senentxu Lanceros-Méndez **Advanced hybrid materials for printed and solid-state batteries: improving performance and sustainability** *BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain* *IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain* *Centro de Física, Universidade do Minho, 4710-057, Braga, Portugal*
10:20-10:45	Coffee break
10:45-11:45	**Auditorium 1** Session: **New Materials and Advanced Materials** CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, Dr. Gil Gonçalves ***Plenary Lecture*** Prof. Dr. Binay Kumar **High Performance Perovskite Piezoelectric Crystals and Nanoparticles for Green Energy** *Crystal Lab, Department of Physics & Astrophysics, University of Delhi, India*

11:45-12:15	Session: **New Methods of Modeling Properties Materials Nanotechnology** CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, Dr. Gil Gonçalves ***Plenary Lecture*** Prof. Dr. Vladimir Bystrov **Modeling and computational study of structures and physical properties of hydroxyapatite containing various defects: a review** *Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*	
12:15-12:40	**Auditorium 1** Session: **Micro / Nano Materials** CHAIR: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques ***Keynote talk*** Dr. María Concepción Serrano López-Terradas **(I8)** **Aiming favorable regenerative features at the injured spinal cord by using nanomaterials assembled in 3D scaffolds** *Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Madrid, Spain*	**Auditorium 2** Session: **Nanotechnology** CHAIR: Dr. Gil Gonçalves ***Keynote talk*** Prof. Dr. Alexander N. Titov **(I2)** **Competition between octo- and tetra-coordination of intercalant in transition metal dichalcogenides** *Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, S. Kovalevskaya St. 18, 620219 Yekaterinburg, Russia*
12:40-13:00	***Keynote talk*** Dr. Pankaj Bharmoria **(I10)** **Air Stable Triplet Harvesting in Nanoconfined Domains of Hydrogels and Bioplastics** *Kasper Moth-Poulsen Lab, Department of Applied Chemistry, Chalmers University of Technology, Kemivägen 4, 412 96 Gothenburg, Sweden*	***Keynote talk*** Prof. Dr. Sergey Bozhko **(I13)** **Crystal structure and resistive switching in NiO** *Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, Moscow District, Russia*
13:00-14:00	Lunch	
14:00-14:50	**Auditorium 1** Session: **Ceramics** CHAIRS: Dr. Duncan Paul Fagg, Dr. Gonzalo Guillermo Otero Irurueta ***Plenary Lecture*** Prof. Dr. Gunnar Suchaneck **Synthesis dependence of the conductivity mechanism and the magnetoresistance of SFMO ceramics** *TU Dresden, Solid-State Electronics Laboratory, Dresden, Germany*	

	Auditorium 1	**Auditorium 2**
14:50-15:15	Session: **New Materials and Advanced Materials** CHAIR: Dr. Duncan Paul Fagg ***Keynote talk*** Prof. Dr. Dmitry Karpinsky **(I1)** **Phase transitions in BiMnO3+δ driven by cations vacancies and temperature** *Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus*	Session: **Thin films** CHAIR Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Dr. Fábio G. Figueiras **(I21)** **Ferroelectricity in epitaxially strained rhombohedral ZrO2 thin films** *IFIMUP & Department of Physics and Astronomy, Sciences Faculty, University of Porto, R. Campo Alegre 687, 4169-007 Porto, Portugal*
15:15-15:35	***Keynote talk*** Prof. Dr. Allisson SAITER-FOURCIN **(I17)** **Nanoscale crystallization mechanisms in a GeSSbCsCl glass-ceramic and relationships with mechanical and optical properties** *Normandie Univ, UNIVROUEN, INSA Rouen, CNRS, Groupe de Physique des Matériaux, 76000 Rouen, France*	Anastasiya Bozhedomova **(O13)** **Investigation of the crystallization kinetics for thin film of phase change memory material on the basis of $GeSb_2Te_4$** *National Research University of Electronic Technology, 124498 Moscow, Russia*
15:35-16:00	Coffee break	
16:00-16:25	Session: **Micro / Nano Materials** Dr. Duncan Paul Fagg ***Keynote talk*** Prof. Dr. Cicero R. Cena **(I12)** **Solution blow spinning as a versatile technique for nanofibers production: an overview** *UFMS – Universidade Federal do Mato Grosso do Sul, Campo Grande-MS, Brasil*	Session: **Thin films** CHAIR Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Dr. Peter Mozhaev **(I15)** **Re-orientation of tilted-axes graphoepitaxial fluorite films towards small-index crystallographic planes** *Valiev Institute of Physics and Technology of Russian Academy of Sciences , Moscow, Russia*
16:25-16:45	Session: **Sensor Materials** CHAIR: Dr. Duncan Paul Fagg Gurjeet Kaur **(O27)** **2-D nanomaterials-based biosensor for Aflatoxin detection** *Academy of Scientific and Innovative Research(ACSIR),Ghaziabad,201002, India; CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C Chandigarh, 160030, India*	Session: **Nanotechnology** CHAIR Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Prof. Dr. Paula Ferreira **(I4)** **Hydrothermal synthesis of barium titanate nanoparticles using a conventional oven and a microwave-assisted reactor** *CICECO – Aveiro Institute of Material, University of Aveiro, Department of Materials and Ceramic Engineering, 3810-193 Aveiro, Portugal*

16:45-17:05	Session: **Sensor Materials** CHAIR: Dr. Duncan Paul Fagg Pallavi Sharma **(O19)** **Polyurethane/ZnS:Mn blended Thin Film for Piezo-luminescence Sensing** *Central Scientific Instruments Organization (CSIR-CSIO), Sector 30 C, Chandigarh,160030, India*	Session: **Thermal Engineering Theory and Applications** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Prof. Dr. Abdelkadir Belhadj **(I18)** **Insights into multiscale rotating machinery R&D: from macro to nano** *DC Engineering & Project Management, Sonatrach, Algiers, Algeria; Computational Mechanics Laboratory, Faculty of Technology, University of Tlemcen, Tlemcen, Algeria*
17:05-17:30	Irina Voloschuk **(O12)** **Formation of Ohmic contacts to the thick films on the basis of Bi_2Te_3 solid solution prepared by screen printing** *National Research University of Electronic Technology , Zelenograd, Moscow, Russia*	Session: **Manufacturing, Virtual Manufacturing and Simulation** CHAIR Dr. Gonzalo Guillermo Otero Irurueta Miguel Fernandes **(O24)** **Finite Element Method Analysis of Two Carbon Fiber Reinforced Polymer Propellant Tanks using Different Manufacturing Methods** *Aerospace Sciences Department, University of Beira Interior. Convento de Sto. António. 6201-001 Covilhã. Portugal*
17:30-17:55	Prof. Dr. Hanna Bandarenka **(O47)** **Fabrication and simulation of electrodynamic properties of ZnO nanowires coated with Ag beads for sensing applications** *National Research University of Electronic Technology, Zelenograd, Moscow, Russia; Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus*	Session: **Optical/Electronic/Magnetic Materials** CHAIR Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Dr. Elena Borisenko **(I26)** **CrNb3S6 Single Crystals Grown by Gas Transport Method** *Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, Moscow District, Russia*
17:55-18:15	Session: **Nanotechnology** CHAIR: Dr. Duncan Paul Fagg Prof. Dr. Mohammed Sanni Haruna **(O30)** **Co-crystal synthesis,characterization and antimycobacterial study of cocrystals of oleanolic acid with isoniazid** *National Agency for Science and Engineering Infrastructure, Idu Industrial Layout, Karimu, FCT, Abuja, Nigeria*	Session: **Manufacturing Process and Mechanical Enginnering** CHAIR Dr. Gonzalo Guillermo Otero Irurueta Asmae Tafraouti **(O3)** **Micro-Electrical Discharge Machining (µEDM): Effect of physical and electrical parameters on crater size** *Institut des Nanotechnologies de Lyon, UMR 5270 CNRS INSA ECL UCB CPE. Université Claude Bernard Lyon1, 43 Bd du 11 Novembre 1918, Villeurbanne Cedex, France*

July 8, 2021 (Thursday)

4th International Conference on Nanomaterials Science and Mechanical Engineering (4th ICNMSME-2021) (*online*)

9:00-9:45	**Auditorium 1** Session: Session: **New Materials and Advanced Materials** CHAIRS: Dr. Gonzalo Guillermo Otero Irurueta, Prof. Dr. Dmitry Karpinsky ***Plenary Lecture*** Prof. Dr. Marc Georg Willinger **Dynamics at catalytically active interfaces: from the simple to the complex** *Scientific Center of Optical and Electron Microscopy, ScopeM, ETH Zürich, Otto-Stern-Weg 3, 8093 Zürich, Switzerland*	
9:45-10:10	**Auditorium 1** Session: **New Materials and Advanced Materials** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Prof. Dr. Neeraj Panwar **(I11)** **Optical and magnetocaloric properties of $HoCr_{0.5}Mn_{0.5}O_3$ compound** *Department of Physic, Central University of Rajasthan, Bandarsindri, Ajmer, Rajasthan 305817, India*	**Auditorium 2** Session: **Biomaterials** CHAIR Prof. Dr. Dmitry Karpinsky ***Keynote talk*** Prof. Dr. Vladimir Bystrov **(O10)** **Structural and physical properties of Sr-substituted hydroxyapatite: modeling and experiments** *Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*
10:10-10:30	Coffee break	
10:30-10:55	Session: **New Materials and Advanced Materials** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta ***Keynote talk*** Prof. Dr. Radheshyam Rai **(I3)** **Dielectric relaxations and dielectric response in multiferroic Gadolinium doping $La_{0.665}Bi_{0.33}Ba_{0.005}A_xMn_{1-x}O_3$ ceramics** *Eternal Univ, Dept Phys, Akal Coll Basic Sci, Sirmour, Himachal Prades, India*	Session: **Nanotechnology** CHAIR: Prof. Dr. Dmitry Karpinsky ***Keynote talk*** Prof. Dr. Gabriela Simone Lorite Yrjänä **(I16)** **Carbon nanotubes boost cell modulation** *Microelectronics Research Unit, University of Oulu, Finland*

10:55-11:20	***Keynote talk*** Prof. Dr. Svetlana G. Titova **(I6)** **Double manganites of rare earth elements: double enchancement of structure and magnetismo** *Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Amundsen St. 101, 620016 Yekaterinburg, Russia*	***Keynote talk*** Prof. Dr. Denis Alikin **(I7)** **Exploring of the material internal electric field from the charged defects by the switching spectroscopy piezoresponse force microscopy** *School of Natural Sciences and Mathematics, Ural federal university, Ekaterinburg, Russia*
11:20-11:45	Session: **New Materials and Advanced Materials / Metal alloy Materials** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta Indra Bahadur Bhandari **(O42)** **Temperature-Dependent Mixing Behaviors of Bi -Mg Liquid Alloys** *Central Department of Physics, Tribhuvan University, Kirtipur, Nepal*	***Keynote talk*** Dr. Maxim Ivanov **(I24)** **Mechanisms of nucleation, growth, and stabilization of local ferroelectric states in organic piezoelectrics** *Department of Materials and Ceramic Engineering & CICECO – Aveiro Institute of Materials, University of Aveiro, Portugal*
11:45-12:05	Session: **New Materials and Advanced Materials** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta Deepanshu Bhatt **(O18)** **Solvothermal synthesis of MIL-125(Ti) Metal Organic Framework and Investigating its photocatalytic activity under visible light in presence of H_2O_2** *Central Scientific Instruments Organization (CSIR-CSIO), Sector 30 C, Chandigarh,160030, India; Academy of Scientific and Innovative Research, CSIR-CSIO, Sector 30 C, Chandigarh,160030, India*	Mara Chiricotto **(O32)** **The role of long-range electrostatic interactions and local topology of the hydrogen bond network in the wettability of fully and partially wetted single and multilayer** *Department of Chemical Engineering and Analytical Science, The University of Manchester, Oxford Road, M13 9PL, Manchester, United Kingdom*
12:05-12:30	Session: **Biomaterials** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta Muhammad Sagir Abubakar **(O36)** **Thermoresponsive, pH and redox-sensitive polymer capsules as drug carriers** *Faculty of Chemistry, Biological and Chemical Research Center, University of Warsaw, Zwirki i Wigury 101, Warsaw, 02-089, Poland*	***Keynote talk*** Dr. Suresh Kumar Jakka **(I25)** **Rare earth doped thermographic phosphors for non-contact temperature sensing** *I3N-Department of Physics, University of Aveiro, Aveiro, Portugal*

12:30-12:50	Dayana L. Guzmán Sierra **(O6)** **Electromechanical characterization of chitosan-based films** *Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Portugal*	Dr. Victor Olugbenga Fadipe **(O31)** **Co-cryatal synthesis,characterization, antimycobacterial and cytotoxicity study of cocrystals of betulinic acid with isoniazid** *Federal Ministry of Science and Technology, Federal Secretariat, FCT, Abuja, Nigeria*
12:50-14:00	Lunch	
14:00-15:00	**Auditorium 1** Session: **New Materials and Advanced Materials** CHAIRS: Dr. Gil Gonçalves, Dr. Francisco Loureiro ***Plenary Lecture*** Prof. Dr. Philip LeDuc **Nature's Unifying Theories and How They Can Be Used for Good** *Departments of Mechanical Engineering, Biomedical Engineering, Computational Biology, and Biological Sciences Carnegie Mellon University, USA*	
15:00-15:25	**Auditorium 1** Session: **2D materials: graphene and others** CHAIR: Dr. Gil Gonçalves Prof. Dr. Vikram Uttam Pandit **(O28)** **Water Pollution control & Hydrogen Production using 2D- Photocatalyst: 6, 13-Pentacenequinone (PQ)** *Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India*	**Auditorium 2** Session: **Optical Materials/Electronic Materials/Magnetic Materials** CHAIR: Dr. Francisco Loureiro Harmeet Kaur **(O25)** **A luminescent DPA@Zn-MOF composite for plausible applicability in Light Emitting Devices** *CSIR-Central Scientific Instrument Organisation (CSIR-CSIO), Chandigarh 160030, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India*
15:30-16:00	Coffee break	
16:00-16:25	Session: **2D materials: graphene and others** CHAIR: Dr. Gil Gonçalves Justyna Niewiadomska-Kaplar **(O8)** **New Way of Conceiving the Structure of Graphene** *Scientific Publishing House Tab, lungotevere degli Anguillara 11, 00153 Rome, Italy*	Session: **Materials Science: Ceramics** CHAIR: Dr. Francisco Loureiro Daniela Lopes **(O23)** **Prospects of metallurgical waste valorisation by the electroreduction of $Fe_{2.3}Mg_{0.7}O_4$ ceramics to Fe** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*

<table>
<tr><td>16:25-
16:50</td><td>Session: Organometallic Compounds
CHAIR: Dr. Gil Gonçalves

Dr. Rayya Al Balushi (O5)
Conjugated Poly(metalla-yne)s for New Materials Applications
Department of Basic Science, College of Applied and Health Sciences, A’ Sharqiyah University, Ibra 400 , Oman</td><td>Session: Nanotechnology
CHAIR: Dr. Francisco Loureiro
Keynote talk

Dr. D. Pukazhselvan (I27)
Facile strategies for nanoconfinement of magnesium hydride for hydrogen storage
TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal</td></tr>
<tr><td>16:50-
17:00</td><td colspan="2">Coffee break</td></tr>
<tr><td rowspan="2">17:00-
18:30</td><td colspan="2">Evening Poster Sessions</td></tr>
<tr><td>Auditorium 1

CHAIR: Dr. Gil Gonçalves

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CHAIR: Dr. Francisco Loureiro

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July 9, 2021 (Friday)

4th International Conference on Nanomaterials Science and Mechanical Engineering (4th ICNMSME-2021) (*online*)

	Auditorium 1	**Auditorium 2**
9:00-9:20	Session: **Nanotechnology** CHAIR: Denis Alikin Vsevolod Mararov **(O46)** **Intercalation of C60 fullerite films by yttrium atoms** *Institute of Automation and Control Processes FEB RAS, 690041 Vladivostok, Russia*	Session: **Composite Materials** CHAIR: Prof. Dr. Neeraj Panwar ***Keynote talk*** Pratik V. Shinde, Prof. Dr. Manoj Kumar Singh **(I14)** **Synergistic Effects of $MoS_2/NiFe_2O_4$ Nanocomposites for High-Performance Energy Conversion and Storage Applications** *Centre for Nano and Material Sciences, Jain University, Jain Global Campus, Jakkasandra, Ramanagaram, Bangalore-562112, Karnataka, India* *Department of Physics under School of Engineering and Technology (SOET), Central University of Haryana (CUH), Mahendergarh- 123031, Haryana, India*
9:20-9:40	SUNG JUN KIM **(O20)** **Ferroelectric polymer based neuromorphic device** *Department of Semiconductor and Display Engineering, Sungkyunkwan University, Suwon 16419, South Korea*	Session: **Ceramics** CHAIR: Prof. Dr. Neeraj Panwar Milan Vukšić **(O11)** **Two-Step Sintering of alumina with the addition of waste alumina powder** *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, Ivana Lučića 1, 10000 Zagreb, Croatia*
9:40-10:00	Session: **Manufacturing Processes and Mechanical Engineering** CHAIR: Denis Alikin SUNG JUN KIM **(O21)** **A study on the streak patterns of the spin coating process** *Department of Semiconductor and Display Engineering, Sungkyunkwan University, Suwon 16419, South Korea*	Session: **Ceramics, fuel cells** CHAIR: Prof. Dr. Neeraj Panwar Laura Holz **(O41)** **$Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ as electrocatalyst for the electrochemical promotion of N_2O reduction** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*

10:00-10:20	Session: **Advanced nanomaterials and sensors** CHAIR: Denis Alikin Monika Nehra **(O7)** **Fluorescent Nanomaterials-based Optical Sensors for Detection of Environmental Contaminants** *Department of Mechanical Engineering, UIET, Panjab University, Chandigarh, 160014, India*	Session: **Composites** CHAIR: Prof. Dr. Neeraj Panwar Martina Kocijan **(O2)** **The efficient solar-light-driven photocatalytic performance of hybrid reduced graphene oxide/TiO_2/graphitic carbon nitride composites for organic pollutant degradation** *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, Ivana Lučića 1, 10000 Zagreb, Croatia*
10:20-10:40	Session: **Nanotechnology** CHAIR: Denis Alikin Fahmida Sharmin **(O34)** **Photodegradation pathways of Rhodamine B over Gd doped $BiFeO_3$ nanoparticles under solar irradiation** *Nanotechnology Research Laboratory, Department of Physics, BUET, Dhaka-1205, Bangladesh*	Pinki Repaswal **(O26)** **Nostoc sp. immobilized rGO-PPy nanocomposite based photoanode for bio electricity generation in non-mediated bio photovoltaic cell** *Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C, Chandigarh, 160030, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India*
10:40-11:00	Md. Shahjahan Ali **(O35)** **Synthesis and optoelectronic characterizations of Cesium Tin Chloride ($CsSnCl_3$) perovskite nanocrystals** *Nanotechnology Research Laboratory, Department of Physics, Bangladesh University of Engineering and Technology, Dhaka-1205, Bangladesh*	Session: **Materials Science: Ceramics** CHAIR: Prof. Dr. Neeraj Panwar Kiryl Zakharchuk **(O22)** **Fabrication and microstructure optimization of highly porous $BaZr_{0.85}Y_{0.15}O_3$ ion-conducting ceramics** *CICECO - Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
11:00-11:20	Coffee break	

	Auditorium 1	**Auditorium 2**
	Session: **New Methods of Modeling Properties Materials** CHAIR: Denis Alikin	Session: **Ceramics** CHAIR: Prof. Dr. Neeraj Panwar
11:20-11:50	***Keynote talk*** Dr. José Coutinho **(I5)** **Identification of the M-center in 4H-SiC as a carbon self-interstitial** *I3N & Department of Physics, University of Aveiro, Portugal*	***Keynote talk*** Prof. Dr. Andrei Kovalevsky **(I9)** **Specific microstructural effects on the performance of thermoelectric oxides** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal*
	Session: **Nanotechnology** CHAIR: Denis Alikin	Session: **New Energy Materials** CHAIR: Prof. Dr. Neeraj Panwar
11:50-12:10	Dr. Leon Avakyan **(O37)** **RDF-recognition of PtCu bimetallic nanoparticle architecture** *Faculty of Physics, Southern Federal University, 5 Zorge St., Rostov-on-Don, 344090 Russia*	Dr. Francisco Loureiro **(O43)** **Magnesium hydride-added titania anode for Li-ion battery** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*
	Session: **Micro / Nano Materials** CHAIR: Denis Alikin	Session: **Material Science (New Energy Materials)** CHAIR: Prof. Dr. Neeraj Panwar
12:10-12:30	Dr. Ekaterina Paramonova **(O38)** **Hybrid density functional study of iron impurities in hydroxyapatite** *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, Pushchino, 142290, Russia*	Vishal Shrivastav **(O16)** **Zinc based Metal-Organic Framework Derived Zinc-Blende Nanoparticles for Supercapacitor Applications** *CSIR-Central Scientific Instrument Organisation (CSIR-CSIO), Chandigarh-160030, India*
	Session: **New Materials and Advanced Materials** CHAIR: Denis Alikin	Session: **Hydrogen and Fuel Cell Science** CHAIR: Prof. Dr. Neeraj Panwar
12:30-13:00	***Keynote talk*** Dr. Svitlana Kopyl **(I19)** **Emergent piezoelectric materials based on self-assembled peptides: application prospects** *Department of Physics & CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal*	Dr. Sergii Sergiienko **(O14)** **MXene-containing composite electrodes for hydrogen evolution** *Department of Materials and Ceramics Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*
13:00-14:00	Lunch	

14:00-14:45	**Auditorium 1** Session: **Thin Films** CHAIRS: D. Pukazhselvan, Dr. Duncan Paul Fagg ***Plenary Lecture*** Prof. Dr. Eudes Borges de Araujo **Defect control and its implications in bismuth ferrite thin films** *Sao Paulo State University (UNESP), School of Natural Sciences and Engineering, Department of Physics and Chemistry, 15385-000 Ilha Solteira, Sao Paulo, Brazil*	
14:45-15:05	**Auditorium 1** Session: **Nanotechnology** CHAIR: D. Pukazhselvan Chandra Shekhar Maurya **(O1)** **Magnetic Field, Heat Transfer and Rheological Analysis of a Magnetorheometer using Finite Element Method** *Research Scholar, Department of Mechanical Engineering, Indian Institute of Technology, Patna, 801103, India*	**Auditorium 2** Session: **Hydrogen and Fuel Cell Science** CHAIR: Duncan Paul Fagg Maksim Kamaleev **(O48)** **Increasing the photoactivity of titanium oxide nanotubes by heat treatment in glycerin** *National Research University of Electronic Technology, Moscow, Russia*
15:05-15:30	***Keynote talk*** Dr. S. Shanmuga Sundari **(I28)** **YAG:Ag nanophosphors – Synthesis and Characterization** *Department of Physics, PSGR Krishnammal College for Women, Coimbatore, India-641004*	Session: **New Energy Materials** CHAIR: Duncan Paul Fagg ***Keynote talk*** Dr. Sergey Luchkin **(I23)** **Nanoscale imaging of functional properties of perovskite solar cell using atomic force microscopy** *Skolkovo Institute of Science and Technology, Moscow, Russia*
15:30-16:00	Coffee break	
16:00-16:20	Session: **New Materials and Advanced Materials** CHAIR: D. Pukazhselvan ***Keynote talk*** Dr. Pavel Zelenovskii **(I29)** **Raman study of ammonia thermal diffusion in diphenylalanine nanotubes** *Department of Chemistry & CICECO–Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*	Svetlana Pereverzeva **(O49)** **Development of a dispersion preparation process based on Al-Ni-FeO_x nanopowders for Direct Ink Writing of energetic materials** *National Research University of Electronic Technology, Bld.1, Shokin Square, Zelenograd, Moscow, Russia, 124498; Scientific-Manufacturing Complex "Technological Centre", Off. 7237, Str. 7 Bld.1, Shokin Square, Zelenograd, Moscow, Russia, 124498*

16:20-16:40	Rachel Sully **(O9)** **Nanoparticle-Infused-Biodegradable-Microneedle Technology for Skin Cancer Treatment** *Medway School of Pharmacy, Universities of Greenwich and Kent, Anson Building, Central Avenue, Chatham ME4 4TB, U.K*	Session: **Hydrogen and Fuel Cell Science** CHAIR: Duncan Paul Fagg Dr. Sergey Mikhalev **(O33)** **Antimony-lead melts for high temperature electrochemical applications** *TEMA-NRD, Mechanical Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal*
16:40-17:05	***Keynote talk*** Dr. Indrani Coondoo **(I20)** **$(BaCa)(ZrTi)O_3$ lead-free piezoelectrics: Recent advancements and perspectives** *Department of Physics & CICECO, University of Aveiro, Aveiro 3810-193, Portugal*	Session: **Ceramics** CHAIR: Duncan Paul Fagg ***Keynote talk*** Dr. Oleksandr Tkach **(I22)** **Antiferrodistortive phase transition in doped strontium titanate ceramics: a role of the perovskite lattice vacancies** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Aveiro, 3810-193, Portugal*
17:05-17:25	Sara Quintana-Sánchez **(O15)** **Bacteria Capture with Magnetic Nanoparticles Modified with Cationic Carbosilane Dendritic Systems** *Dpto. de Química Orgánica y Química Inorgánica, Universidad de Alcalá (UAH), Campus Universitario, E-28805 Alcalá de Henares (Madrid) Spain*	Session: **Nanotechnology** CHAIR: Duncan Paul Fagg Lyubov Gimadeeva **(O44)** **Quantitative measurements of the piezoelectric coefficients using "global-excitation" mode of the piezoresponse force microscopy** *School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia*
17:25-17:45	Sarka Sovova **(O39)** **PHYSICAL CHARACTERIZATION OF SiO_2 NANOFLUID** *Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkynova 464/118, 612 00, Brno, Czech Republic*	Denys Bondar **(O45)** **Nanodiamonds as a treatment for organophosphate poisoning** *Department of Chemistry and Biotechnology, TalTech, Akadeemia tee 15, Tallinn, 12618, Estonia*

17:45-18:05	Priyanshu Goel **(O17)** **Synthesis of High Luminescent and Stable Hybrid Metal-Organic Frameworks and Perovskite Nanocomposite as phosphor for Green LED** *Central Scientific Instruments Organization (CSIR-CSIO), Sector 30 C, Chandigarh,160030, India; Academy of Scientific and Innovative Research, CSIR-CSIO, Sector 30 C, Chandigarh,160030, India*	Session: **Engineering and technology** CHAIR: Duncan Paul Fagg AMRANI Djedjiga **(O4)** **Aerodynamic efficiency analysis of winglet using CFD** *Uniersity of science and technology Mohamed Boudiaf, El Mnaouer Bp1505 Bir El Djir 31000, Oran Algeria*
18:05-18:25	Vanessa C.D. Graça **(O40)** **The influence of ammonolysis temperature and time on synthesis of cubic niobium (oxy)nitride** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*	Session: **Environmental Friendly Materials** CHAIR: Duncan Paul Fagg Dr. Aleksey Lisenkov **(O29)** **Iron electrowinning under alkaline conditions: effects of the current interruptions** *Department of Materials and Ceramic Engineering/ CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal*
18:25-19:00	**Auditorium 1** **Conference Closing Ceremony**	

Poster session

P1	**Corrosion Resistance of Cor-Ten Steel in Different Environments** Tajana Horvat, Vera Rede, Dajana Mikić, Helena Otmačić Ćurković *Department of Binders and Ecology, Institut IGH, JSC, Janka Rakuše 1, 10000 Zagreb, Croatia; Department of Materials, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia; Department of Electrochemistry, Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10000 Zagreb, Croatia*
P2	**Effects of microstructural orientation on bending strength in the longitudinal direction of pedunculate oak** Vera Rede, Sara Essert, Tajana Horvat *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia; Division of Botany, Department of Biology, Faculty of Science, University of Zagreb, Marulićev trg 20/ II, 10000 Zagreb, Croatia; Department of Binders and Ecology, Institut IGH, JSC, Janka Rakuše 1, 10000 Zagreb, Croatia*
P3	**The mechanical behaviour of concrete with chicken feather fibres at high temperature** Sahnoun Ilhem *Laboratoire Matériaux et Durabilité des Constructions (LMDC), Route Ain El bey, Constantine, Algeria*
P4	**Effect of long baffles on forced convection heat transfer over multiple heated blocks** Hamza AMIRAT, Abdelkader KORICHI *University of Yahia Fares, Laboratory of Mechanics, Physics and Mathematical Modeling (LMP2M) Medea, Algeria*
P5	**Cobalt oxyhydroxide nanoflakes-reduced graphene oxide nanocomposite based Electrochemical detection platform for determination of Flunitrazepam in Biological Samples** Garima Chhikara, Abhay Sachdev *Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30-C, Chandigarh, 160030, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India*
P6	**Use of Infrared Temperature Sensor to Estimate the Evolution of Transformation Temperature of SMA Actuator Wires** Maria Clara S. de Castro, Tadeu Castro da Silva *Fluminense Federal University, Rua Passo da Pátria, 156, Niterói RJ, Brazil, 24210-240*
P7	**Measuring Systems for Investigating the Physical Properties of Superconducting Materials** Giorgi Giorganashvili, B. Bendeliani, G. Bokuchava, G. Dgebuadze, I. Metskhvarishvili, E. Sanaia, K. Shamatava, V. Chanturidze *Ilia Vekua Sukhumi Institute of Physics and Technology, Laboratory of Cryogenic Technique and Technologies, 7 Mindeli St., 0186 Tbilisi, Georgia*

P8	**A first-principles study on the electronic and optical properties of Nd_2FeCrO_6 double perovskite** M. D. I. BHUYAN, Subrata Das, M. A. Basith *Nanotechnology Research Laboratory, Department of Physics, Bangladesh University of Engineering and Technology, Dhaka-1205, Bangladesh*
P9	**Free vibration analysis of functionally graded SWNT** AOUINAT Ahmed Lamine, BOUKHALFA Abdelkrim *MECACOMP Laboratory, Faculty of Technology, Abou Bekr Belkaid University, Tlemcen, ALGERIA*
P10	**Experimental and theoretical study of carbon micro- and nano-spheres doped by nitrogen** Leon Avakyan, Aram Manukyan, Daria Tolchina, Ratibor Chumakov, Alexey Emelyanov, Narek Sysakyan, Harutyun Gyulasaryan, Lusegen Bugaev *Southern Federal University, Faculty of Physics, Zorge str.,5, Rostov-on-Don, Russia; Institute for Physical Research, National Academy of Sciences of Armenia, Ashtarak, Armenia; National Research Center "Kurchatov Institute", Moscow, Russia*
P11	**Vibration study of a piezoelectric nano-shaft** Behar Merwan, Boukhalfa Abdelkrim *Department of Mechanical Engineering, Faculty of Engineering, computational mechanics, Tlemcen, Algeria*
P12	**Crystal structure and magnetic phase transitions in $BiFeO_3$ based ceramics driven by high pressure** M.V. Silibin, D.V. Zhaludkevich, S.I. Latushka, A.A. Dronov, A.V. Sysa, K.N. Nekludov, D.V. Karpinsky *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Scientific-Practical Materials Research Centre of NAS of Belarus, 220072 Minsk, Belarus*
P13	**Plasmonic nanostructures based on the metalized porous silicon for SERS** K. Girel, A. Burko, S. Zavatski, N. Khinevich, S. Dubkov, A. Savitsky, D. Novikov, A. Tarasov, H. Bandarenka *Applied Plasmonics Laboratory, Belarusian State University of Informatics and Radioelectronics, 6 Brovka St., 220013, Minsk, Belarus; Swiss Federal Institute of Technology Lausanne, 11 Station St., CH-1015, Lausanne, Switzerland; Department of Physics, Kaunas University of Technology, Studentų; St. 50, Kaunas, 51368, Lithuania; Institute of Advanced Materials and Technologies, National University of Electronic Technology, 1 Shokin Sq., Zelenograd, Moscow, 124498, Russia*
P14	**Local electrophoretic deposition of TiO_2-CuO_x nanocomposites for gas sensors** L. Sorokina, N. Litovchenko, R. Ryazanov, E. Lebedev *National Research University of Electronic Technology "MIET", 124498, Moscow, Russia; Scientific Manufacturing Complex "Technological Centre", 124498, Moscow, Russia*

P15	**Influence of Swift Heavy Ag^{7+} ion irradiation on room temperature ferroelectric Triglycine Sulphate single crystal.** V.C. Bharath Sabarish,G. Ramesh Kumar,A. Durairajan,M. P. F. Graça, M.A. Valente, S. Gokulraj *Departement of Physics, University College of Engineering Arni -Thatchur 632 326, India; 3N-Aveiro, Department of Physics, University of Aveiro, Aveiro 3810 193, Portugal; Department of physics, C.Kandasamy Naidu College for Men Chennai, India*
P16	**Effect of calcination temperature on vibrational and optical absorption properties of $BiFeO_3$ – Graphene and $BiFeO_3$ –MWCNT Nanocomposites** C. Anandaraj, A. Durairajan, M.P. Graça, M.A. Valente, S. Gokul Raj, G. Ramesh Kumar *Department of Physics ,University College of Engineering Arni-Thatchur 632 326,India; I3N-Aveiro-Department of Physics ,University of Aveiro, Aveiro 3810193 Portugal; Department of Physics, C. Kandaswami Naidu College for Men Chennai, India*
P17	**Temperature evolution of the crystal structure and piezoelectric response in BiFeO3-BaTiO3 solid solutions on the rhombohedral-pseudocubic phase boundary** A.S. Abramov, D.O. Alikin, A.P. Turygin, A. Zheludkevich, D. Zheludkevich, A. Pakalniškis, R. Skaudžius, A.L. Kholkin, D. Karpinsky *School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia; Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus; Institute of Chemistry, Vilnius University, Vilnius, Lithuania; Department of Physics & CICECO – Aveiro Institute of Materials, University of Aveiro, Portugal*
P18	**Investigation of the optimal method for applying the analyte R6G to the SERS substrate based on silver nanoparticles** N.Mineeva, S.Dubkov, A. Savitsky, K. Girel, A.Burko, S. Zavatsky, D.Novikov, A.Tarasov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Belarusian State University of Informatics and Radioelectronics, 220013 Minsk, Belarus*
P19	**Detection of Trimethylamine Oxide by Surface Enhanced Raman Spectroscopy** D.Novikov, H.Bandarenka, A.Burko, S.Zavatsky, K. Girel, S.Dubkov, D.Gromov, A. Savitsky, A.Tarasov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Belarusian State University of Informatics and Radioelectronics, 220013 Minsk, Belarus*
P20	**Conversions of CO2 and CH3OH on the TiO2 surface under ultraviolet radiation and high pressure** S. Dubkov, A. Overchenko, L. Sorokina, D. Gromov, A. Tarasov, T.Maniecki, A.Shtyka, R. Ciesielski *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Lodz University of Technology, 90-924 Lodz, Poland*
P21	**Development of approaches to the formation of TiO2 nanowires for sensitive elements of biosensors** S. Dubkov, A. Tarasov, D. Gromov, D. Vu Van *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia*

Plenary lectures

Nature's unifying theories and how they can be used for good

Philip LeDuc

Departments of Mechanical Engineering, Computational Biology, Biomedical Engineering, Electrical and Computer Engineering, and Biological Sciences
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I have always been interested in examining whether seemingly unconnected areas of my life actually have intersections. For example, two areas that have always interested me are the mechanics of machines such as taking apart lawn mowers in my youth and the wonders of nature. While they seem unconnected, I wonder what are their commonalities, which has lead me to work on this intersection for almost 2 decades toward unifying theories between them. Here I will present how my lab has been looking for nature's unifying theories that are threaded throughout life. My lab approaches this by envisioning different biological organisms as "systems" and is examining how these unconnected systems intersect. We use our approaches as engineers for investigating these systems in nature looking for unifying principles with some of the same fundamental approaches used on machines such as planes, trains, and automobiles. The biological systems range from mammalian cells to microorganisms to plants (e.g. neurons, magnetic bacteria, energy generating bacteria, *Xenopus laevis*, stem cells) and we apply principles from mechanical engineering fields (e.g. solid mechanics, control theory, fluidics, heat transfer, design) to understand how these principles may apply across diverse nature-based systems. In addition, I will present in this talk our approaches of using solid mechanics in areas such as cell mechanotransduction. We pursue these goals through developing and utilizing unique custom-built systems as well as nanotechnology, microtechnology, and computational biology. These intersections are especially fascinating to me as biological systems have evolved for distinct reasons (the "initial and boundary conditions" are different). In addition, as an engineer, I truly am interested in building new systems from the knowledge that we obtain in a similar thought process as we use information to build new systems. Thus, I will also present how our lab thinks about nature-inspired design principles at the molecular and cellular levels to work toward generating novel approaches for contributing to technology development and medical applications.

Dynamics at catalytically active interfaces: from the simple to the complex

Marc Willinger

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Heterogeneous catalysis is concerned with the study of reactions and dynamics at interfaces. The active catalyst is involved in bond breaking and bond making and thus, experiences a constant change in surface coverage due to adsorption, reaction, and desorption of species. The transfer of charge, energy and, eventually, chemical species at the surface of the catalyst induces a response that feeds back into the reaction. If well played, the concerted dynamics emerging in the interaction between reactive gas-phase and active catalyst give rise to complex structural and temporal dynamics that can be associated to catalytic function.
Over the last years, we have investigated the dynamic behavior of catalytically active metals by a combination of in-situ and operando scanning- and transmission electron microscopy (SEM and TEM, respectively). This multi-scale approach allows both, the study of collective large-scale dynamics from the mm to the nm scale, as well as studies of atomistic processes on individual active metal nanoparticles. We have observed the propagation of chemical waves and formation of dissipative structures during hydrogenation of nitrogen dioxide on platinum foils [1], as well as complex redox transformations of metal catalysts in model redox reactions [2,3]. As a next step, we increased the complexity from simple metals to supported metal catalysts. Using the prototype titania supported platinum catalyst, we studied effects related to a strong metal-support-interaction (SMSI). Starting with a description of the catalyst under oxidizing conditions based on a combination of in-situ TEM imaging and X-ray spectroscopy [4], we are now moving forward and hopefully, reveal the underlying atomistic interactions that are at play under reactive conditions and responsible for the superior catalytic activity of supported metal catalysts.
The aim of my presentation is to demonstrate the potential of In-situ and operando electron microscopy and highlight the importance of observing processes while they are happening.

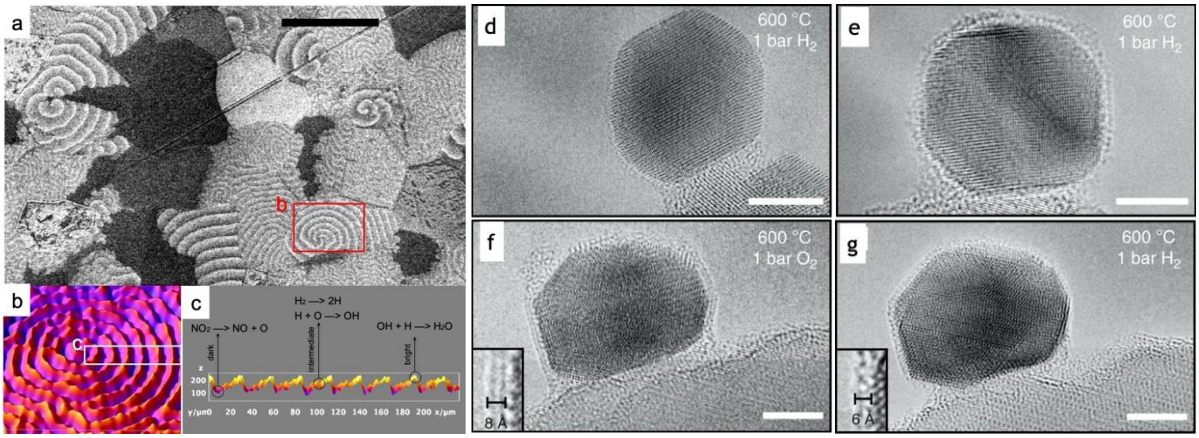

Figure 1: (a-c) Contrast variations caused by propagating chemical waves as revealed by in-situ SEM during NO_2 hydrogenation on a polycrystalline Pt foil [1]. Examples of in-situ TEM are shown in panels (d-g): A platinum particle on a titania support in the first exposure to H_2 at 600 °C (d, e) and the subsequent atmosphere change to O_2 at 600 °C (f), and back to H2 (g). Scale bar: 5nm [2].

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Modeling and computational study of structures and physical properties of hydroxyapatite containing various defects: a review

V.S. Bystrov [1, *], E.V. Paramonova [1], S.V. Filippov [1] , A.V. Bystrova [1,2], L.A. Avakyan [3] , J. Coutinho [4]

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The modeling and computational study of the hydroxyapatite (HAP), containing different defects are presented in this review. The dependence of the structural and physical properties of HAP on the presence of various defects in their structure is considered in details [1-3].

Hydroxyapatite (HAP) is a well-known material which actively used in various fields of medicine (bone and dental implantology) and nanotechnology. Recently, new HAP applications in ecology and photocatalytic processes, in the fight against cancer (as a means of targeted drug delivery and local hyperthermia) and even when producing hydrogen for power engineering were investigated. However, all features of the structure and properties of HAP, especially HAP defects, are not fully understand yet. This fact hinders HAP world-wide using both in traditional and newly discovered fields.

Mostly the HAP properties, containing the defects, are determined by the presence of various structural imperfections such as oxygen and hydroxyl vacancies, interstitials and substitutions of ions, atoms and atomic groups in the structure of HAP. Recently it was possible to establish using modern methods of density functional theory (DFT) and the corresponding new software tools in modeling and computer researches of the properties of HAP structures with these various defects types. It was established that the band gap Eg of an ideal (defect-free) HAP lattice is about Eg ~ 7 - 8 eV, which significantly exceeds the experimentally observed values for synthesized and used in practices HAP samples (Eg ~ 4 - 5 eV) [2]. The results of these recent modeling researches of HAP structure with defects have convincingly shown that the deviations of the band gap width of the calculated data from the registered in the experiments values are produced namely by the presence of defects in the HAP structure.

In these calculations of the oxygen vacancies, (from the PO_4 and OH groups, with various symmetry) and OH-group vacancies in HAP structure are investigated using the modern new types of DFT hybrid functionals and many-body perturbation theory. The approximation of the dynamically screened single-particle Green's function, were developed and applied to consider the optoelectronic properties of such HAp with defects. The use of a mixture of (semi) local and exact exchange in the exchange-correlation functional is considered, which leads to an improvement in the energy band structure. These studies of the structural and electronic properties of oxygen vacancies, using hybrid DFT functionals, are carried out in large HAP supercells within the plane-wave

formalism and in the generalized gradient approximation. This study was shown that under equilibrium conditions, vacancies arise either in the form of a simple vacant oxygen site (in the neutral charge state) or in the form of extended structures occupying several crystalline moieties (in the double plus charge state) [3]. It should be noted that these new structural defects can play an important role in changing the properties of the electrically charged HAP.

In addition, the study of the transitions between the energy levels of such defects showed that the transition of electrons from the top of the valence band to the donor state of the vacancy includes a zero-phonon transition of 3.6–3.9 eV. Most likely namely this mechanism explains the onset of absorption at 3.4–4.0 eV in the experimental observation of photocatalysis using HAP under persistent UV illumination.

Previously, the role and influence of defects such as substituted atoms/ions in the structure of HAP were also established (but using other DFT approximations and software) [1]. The review analyzes these results too and suggests further research using modern hybrid DFT functionals study in this important direction. Special interest for practical applications has such defects as substitution of iron ions (Fe^{2+}, Fe^{3+}), strontium ions, and other atoms.

The obtained results of modeling and calculations HAP, containing various defects, make it possible to investigate, find out, and then predict which defect types cause certain physical properties of HAP, and make it possible to determine the conditions for their production for practical applications. The study was supported by a grant Russian Science Foundation (RSF) No. 21-12-00251.

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Defect control and its implications in bismuth ferrite thin films

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The bismuth ferrite ($BiFeO_3$) is a prototype multiferroic material at room temperature, with high Curie temperature (T_C ~ 1103 K) and Néel temperature (T_N ~ 643 K). Due to its excellent ferroelectric properties and the possibility of coupling their ferroelectric and magnetic properties, the $BiFeO_3$ emerges as a promising material for developing the next generation of multifunctional devices. However, the problematic control and incomplete understanding of extrinsic and chemical defects in this multiferroic have been significant obstacles limiting its practical technological application. Despite several approaches taken to solve these problems, there is consensus in the literature that different types of defects lead to modifications on the electrical properties of the $BiFeO_3$, including a large leakage current at room temperature. Impurities, bismuth vacancies, oxygen vacancies, and secondary phases induced by small fluctuations in stoichiometry occurring during growth are common defects observed. $BiFeO_3$ thin films with specific and desired characteristics are challenging in this scenario, depend on the used method, and require meticulous tuning of growth parameters. Among several physical and chemical techniques, the chemical solution route possesses precise control of stoichiometry and homogeneous deposition. In this talk, we review the origin of different defects in $BiFeO_3$ thin films prepared by chemical solution route and its implications on their physical properties. The importance of controlling the processing parameters during the growth and the impact of defects on the electrical properties will be discussed [1,2]. Finally, recent results on $BiFeO_3$ thin films with different Bi:Fe ratios will also be presented. These results indicate that the mechanism behind the leakage current in these films is probably more intricate and maybe interrelated with complex defects associated with the Bi:Fe ratio than the concentration of oxygen vacancies.

References

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High performance perovskite piezoelectric crystals and nanoparticles for green energy

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Crystals play pivotal role in technological development and in felicitating our daily life. Nature has given us many crystals of excellent, but fixed properties. Therefore, we need to grow crystals of desired materials and properties. In the present talk our recent works on technologically important piezoelectric crystals will be presented.

Piezoelectricity is a unique phenomenon in which by application of force on a piezoelectric material one can generate electric energy. Typical value of piezoelectric charge coefficient (i.e. charge developed per unit force) for some well known materials are 1-2 pC/N for quartz, 2-5 for ZnO, 2-20 for organic materials, around 100 for $BaTiO_3/KNbO_3$, 400 pC/N for PZT, etc. Higher values of piezoelectricity are required for higher efficiency of piezoelectric energy harvestors.

We have grown single crystals of lead based binary perovskite like PMN-PT and lead free NKLN whose piezoelectric charge coefficient are above 1500 pC/N and 500 pC/N, respectively. Single crystals of these materials are grown by flux method and high piezoelectric/ferroelectric /pyroelectric properties have been achieved [1-2]. These crystals are characterized for crystallographic, electrical, mechanical, optical, etc properties. The concept of true/usable/switchable polarization from the P-E loop using PUND and LOGIC treatment will also be discussed. It will be demonstrated that electric energy can be generated by simple finger tapping and that piezoelectric force sensor and energy harvestors can be fabricated using these systems [3-5].

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Advanced hybrid materials for printed and solid-state batteries: improving performance and sustainability

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The constant technological development and the increasing mobility lead to the necessity of new ways of energy generation and storage. Lithium ion batteries are increasingly being used in portable devices and show some advantages when compared to other systems such as nickel-cadmium and nickel-metal, due to higher energy storage, high capacity and higher number of charge-discharge cycles.

The increasing use of those energy storage systems demand a new generation of materials with improved performance, sustainability and fabrication possibilities.

An overview on the main materials and processes being developed for printable and solid state batteries will be provided, with special focus on both performance and sustainability.

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Synthesis dependence of the conductivity mechanism and the magnetoresistance of $Sr_2FeMoO_{6-\delta}$ ceramics

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$Sr_2FeMoO_{6-\delta}$ (SFMO) double perovskite is a promising candidate for room-temperature spintronic applications since it possesses a half-metallic character (with theoretically 100% spin polarization), a high Curie temperature of about 415 K, and a low-field magnetoresistance (LFMR) [1]. A typical synthesis route of SFMO ceramics includes (i) chemical synthesis, for instance by solid state reaction or sol-gel processes, (ii) grinding, (iii) cold pressing, and (iv) long-term annealing at high temperatures in different environment. Annealing below 900°C does not affect the iron/molybdenum B-site ordering. The antisite disorder Fe_{Mo} and Mo_{Fe} is lowest at an optimum synthesis temperature, which amounts to about 1200°C for ceramics long-term annealed under oxygen-deficient conditions, and to about 850°C for SFMO thin films deposited by pulsed laser deposition [1]. Annealing above 1500ºC practically removes all the antiphase boundaries [2]. Consequently, with regard to synthesis conditions, we have to deal not with one, but with very different magnetic materials.

In this work, we analyze the different conductivity and magnetoresistance (MR) mechanisms of SFMO: (i) MR across antiphase boundaries [3], (ii) intergranular MR caused by spin-polarized tunneling [4], (iii) fluctuation induced tunneling in low-temperature post-annealed SFMO ceramics [5], and (iv) MR through $SrMoO_4$ tunneling barriers [6]. We discuss controlled SFMO ceramics fabrication in order to design the magnetic properties of spintronic devices, first of all, magnetic field sensors and magnetoresistive random access memories.

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Invited speakers

I1. Phase transitions in $BiMnO_{3+d}$ driven by cations vacancies and temperature

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Bismuth manganite ($BiMnO_3$) is well known magnetoelectric material with perovskite structure with magnetic transition temperature T_C ~ 102 K [1]. The ferromagnetic order in $BiMnO_3$ is caused orbital ordering, which is destroyed at T ~ 475 K [2]. Magnetic structure of $BiMnO_3$ is determined by positive exchange interactions formed between ions Mn^{3+}, while the type of the exchange interactions strongly depends on orientation of the 3d orbitals of Mn ions as well as geometry of the chemical bonds Mn - O - Mn [3]. The crystal structure and magnetic properties of $BiMnO_3$-based compounds can be significantly modified via chemical doping [4]. Self-doping approach [5] can be used as entirely internal stimulus which causes a modification of the crystal structure and thus changes the magnetic state of the compounds which can facilitate an analysis of the structure-properties relationship.

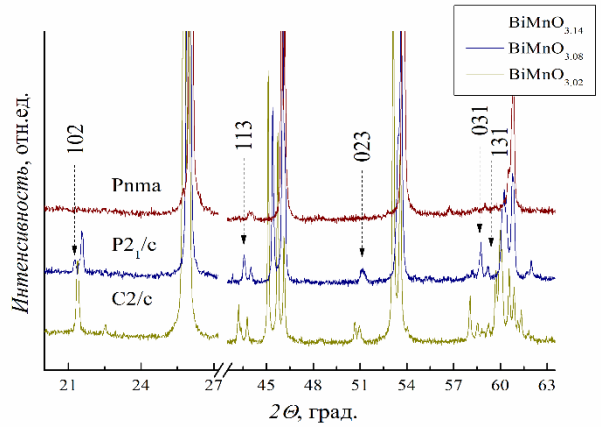

Fig.1. Diffraction patterns of the ceramics $BiMnO_{3+d}$ (d = 0.02, 0.08, 0.14); reflections characteristic for different structural phases are marked.

The XRD results obtained for $BiMnO_{3+d}$ ceramics have shown that an increase in nominal oxygen excess leads to a series of the phase transitions from the monoclinic structure (space group C2/c) to another monoclinic (P21/c) and then the orthorhombic structure (Pnma) through the two-phase regions (Fig. 1). The sequence of the phase transitions is accompanied by a gradual destruction of the orbital ordering which is caused by nonuniform distribution of vacancies of manganese ions throughout the B-sublattice of the perovskite structure.

The research was supported by RSF (#21-19-00386).

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I2. Competition in the distribution of intercalated metals over octahedral and tetrahedrally coordinated positions in intercalate compounds of transition metal dichalcogenides

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Layered transition metal dichalcogenides and their intercalate derivatives exhibit a wide range of physical effects from superconductivity to the state of multiferroics. Positions into the interlayer space octahedrally and tetrahedrally coordinated by chalcogen may be occupied by IV group metal atoms during intercalation. Materials with tetra-coordinated intercalated atoms are of particular interest. In such materials, the formation of a noncentrosymmetric crystal structure is possible. This stabilizes the ferroelectric and/or ordered magnetic state. Such lattices have an increased polarizability, which affects the electron-lattice interaction.

Our investigations of the crystal and electronic structure of intercalates based on dichalcogenides of IV and V groups transition metals show that potential of ionization of the host lattice transition metal determines dominated type of coordination of the guest atom. We discuss the ways to control the ionization potential of the transition metal of the host lattice and the stability of the non-centrosymmetric structures.

The work is supported by RFBR, grant No 20-03-00275.

I3. Dielectric relaxations and dielectric response in multiferroic Gadolinium doping $La_{0.665}Bi_{0.33}Ba_{0.005}A_xMn_{1-x}O_3$ ceramics

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X-ray diffraction pattern of the $La_{0.665}Bi_{0.33}Ba_{0.005}Gd_xMn_{1-x}O_3$ (x = 0.25, 0.45, 0.65) (where x= 0.35, 0.55, 0.75) ceramics with no impurity phases was confirmed. A peak shift (~32°C) was observed in the XRD pattern. Orthorhombic structure was confirmed for x= 0.25 and 0.45 but mixed phase (both orthorhombic and rhombohedra) was confirmed for x= 0.65 from the rietveld refinement of the X-ray diffraction pattern. Average crystallite value decreased with increasing value of Gadolinium doping. The decreasing value of real part of impedance with increasing temperature revealed the semiconducting behavior of the samples. The master curves confirmed the temperature-independent conduction mechanism in all the samples. Z″/Z″ max curves were found to be non-symmetric, implying a non-exponential behavior of the conductivity relaxation. The dielectric spectra of the samples showed negative dielectric behavior at frequencies bellow 10^3 Hz. However at temperatures above 350°C a positive dielectric behavior of the samples was observed. AC conductivity value of the samples was found to increase with increase in temperature indicating the semiconductor behavior of the samples.

I4. Hydrothermal synthesis of barium titanate nanoparticles using a conventional oven and a microwave-assisted reactor

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Barium Titanate (BT) is gaining nowadays a strong interest as a prototype of lead-free ferroelectric and piezoelectric material for a large number of applications ranging from sensors to memories.[1] BT production routes often include long processing times, metal alkoxides precursors, organic solvents, and/or high heating temperatures through methods such as hydrothermal synthesis, sol-gel, coprecipitation, thermal decomposition.[2] These methodologies are not environmentally sustainable and there is a strong need to develop simple, cost-effective and environmentally friendly alternatives [3]. Herein, it is investigated the synthesis of BT nanoparticles by hydrothermal processes using: i) a conventional oven, and ii) a microwave-assisted reactor in order to understand the relationship between the heating system and the structure, morphology/size and final properties. The temperature of 200 °C and 1, 3 and 6 h of reaction were chosen as conditions of study. The obtained nanoparticles were structurally and morphologically characterized by X-ray diffraction, Raman, thermogravimetric analysis, Fourier-transform infrared spectroscopy, scanning and transmission electron microscopy. The piezoelectric properties of the corresponding ceramics were also analyzed. XRD and Raman analyses showed faster BT phase formation for MW samples as well as better defined particles at all three reaction times. The degree of tetragonality was higher with MW procedure, requiring 72 h of hydrothermal treatment in a conventional oven to achieve similar tetragonality. Selected conditions were also applied to investigate the effect of the presence of graphite during the synthesis process on the resulting BT properties.

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I5. Identification of the M-center in 4H-SiC as a carbon self-interstitial

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The identification of self-interstitials in technological crystalline materials, such as semiconductors, have profound repercussions on a wide range of scientific areas. Examples of benefited fields are mass transport, crystal growth, doping and defect engineering in both mature and emerging technologies. Supported on detailed first-principles modeling and junction spectroscopy experiments, we present unambiguous evidence that the M-center in 4H-SiC [1,2] is the carbon self-interstitial [3]. The M-center is a bistable defect whose Deep Level Transient Spectroscopic (DLTS) signal depends on the bias/thermal history of the sample. Spectrum labeled 'A' comprising traps M_1 ($E_c - 0.42$ eV) and M_3 ($\sim E_c - 0.83$ eV), is obtained when the sample is cooled from room temperature under reverse bias. On the other hand, when the DLTS scan is preceded by a gentle annealing at $T > 140$ °C without bias, spectrum 'B' appears, showing up a single emission M_2 ($E_c - 0.63$ eV) [1,2]. The carbon self-interstitial is predicted to adopt different sublattice sites depending on the Fermi level location. In n-type material, double negative C_i in the cubic site is the ground state, whereas under intrinsic conditions (reverse biased n-type 4H-SiC) the defect performs an exothermic jump towards the hexagonal site. The model developed incorporates the observed features of M, including charge states, bistability, annealing, reconfiguration kinetics and electronic transition levels. The observation of a new peak by isothermal DLTS (also accounted for by the C_i model) [3], labeled M_4 ($E_c - 0.86$ eV) and previously postulated as a fourth acceptor transition of the M-center [2], provides an important piece of evidence in the connection between M and the self-interstitial. Our findings represent an important step towards obtaining control over countless solid-state reactions involving self-interstitials in 4H-SiC, including the formation of defects for quantum technologies or the fabrication of more efficient power electronic devices.

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I6. Double-perovskite manganites of rare earth elements: double enhancement of structure and magnetism

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Double-perovskite manganites RBaMn$_2$O$_6$ (R – rare earth element) with ordered alternate stacking of RMnO$_3$/BaMnO$_3$ layers attract a special interest due to the presence of two magnetic phase transitions close to room temperature. The temperatures of magnetic phase transitions in these materials are roughly twice those for non-ordered (R,Ba)MnO$_3$ manganites. Thus, the use of magnetoresistive and magnetocaloric effects associated with magnetic phase transitions in these materials is attractive for practical applications and makes them perspective magnetocalorics and magnetoresistors. For the first time we have fabricated solid solutions with A-site substitution Nd$_{1-x}$Pr$_x$BaMn$_2$O$_6$ and Sm$_{1-x}$Nd$_x$BaMn$_2$O$_6$ and investigated their structural and magnetic properties. The origin of structural phase transition accompanied with the elongation of the a-axis and the contraction of the c-axis was studied by X-ray powder diffraction, X-ray photoelectron spectroscopy (XPS), IR absorption spectroscopy, magnetometry and dynamical mean-field theory (DMFT) for electronic structure calculations. It is found that the structural phase transition is caused by splitting of e_g-doublet states at orbital ordering due to metal-insulator phase transition.

The work is supported by RFBR, grant No 19-29-12013.

I7. Exploring of the material internal electric field from the charged defects by the switching spectroscopy piezoresponse force microscopy

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The monitoring of the charged defect at the nanoscale is vital in many material-science studies of ferroelectrics. Up to date, high-resolution methods to study defects are expensive and demand complicated sample preparation. Here, we showed that switching spectroscopy mode of the piezoresponse force microscopy (SS-PFM) can probe simultaneously ferroelectric properties of the material and electric potential from the charged defects. The complimentary data of the neutron diffraction, X-ray photoelectron spectroscopy, and local time-of-flight secondary ion mass spectrometry data allowed to conclude that SS-PFM achieves outstanding sensitivity to the charge defects above 100 ppm. The evolution of the material inner bias field created by the charged defects during local polarization reversal gives an insight of the ferroelectric polarization retention and interaction of the domain walls and charge defects. The reported results manifest an immense contribution of the charged defect to the surface screening of the depolarization field in ferroelectric materials and open new capabilities to observe and control charged defects at the nanoscale.

The equipment of the Ural Center for Shared Use “Modern Nanotechnology” UrFU was used. The work is supported by the Russian Science Foundation (grant 19-72-10076).

I8. Aiming favorable regenerative features at the injured spinal cord by using nanomaterials assembled in 3D scaffolds

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Graphene-based materials (GBMs) have arisen as promising building block materials for the development of a wide diversity of biomaterials and devices in a plethora of biological scenarios, both *in vitro* and *in vivo*. Even when their biocompatibility continues to be an open debate for scientists, outstanding efforts are prompting their exploration in biomedicine [1]. *In vitro*, GBMs are able to modulate neural cell survival, neurite growth and differentiation [2], electrical signaling and ion channel function [3], to cite a few. However, studies in preclinical models *in vivo* are still limited. Since 2014, our group has focused on the exploration of 3D reduced graphene oxide (rGO) biomaterials as supportive platforms for neural repair at the rat injured spinal cord, exploring both microfibers and porous foams architectures [4,5]. 3D foams are fabricated by using a freeze-casting methodology and microfibers by a hydrothermal process. *In vivo* models included a cervical right hemisection at C6 level and a complete transection at T9 level. Time points under study comprised 10 (subacute), 30 (early chronic) and 120 (late chronic) days. Both systemic and local responses at the injured spinal cord have been examined. From the early time points investigated, rGO biomaterials seem to mediate favorable responses towards the stabilization of the lesion site, evidencing a remarkable infiltration of the 3D structure. In early chronic stages, the formation of vascular structures to nourish the lesion was favored inside the foams, accompanied by neurites growth and immunomodulatory effects on macrophages. Foams in late chronic animals were largely colonized by excitatory neurites and functional blood vessels. Finally, the combination of these 3D rGO biomaterials with a motor training routine significantly impacted immune, vascular and neural features at the injured spinal cord. Our work is proving the beneficial effects that rGO-based 3D biomaterials sustain at the injured spinal cord. Further work is encouraged to take full advantage of the potential of these materials in neural tissue engineering.

This work was funded by the *Agencia Estatal de Investigación and the Fondo Europeo de Desarrollo Regional* (MAT2016-78857-R, AEI/FEDER, UE).

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I9. Specific microstructural effects on the performance of thermoelectric oxides

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Oxide materials possess notable high-temperature and chemical stability, thus representing certain advantages over traditional thermoelectrics. The thermoelectric performance of oxides is strongly affected by the microstructure, often even dominating over the chemical composition effects. Thus, engineering the microstructure in these materials represents a powerful tool towards improving their thermoelectric performance, both in terms of the maximum output and stable operation at elevated temperatures. This work reviews some representative cases observed for the main thermoelectric oxide families, such as ZnO, $SrTiO_3$, $Ca_3Co_4O_9$ and $CaMnO_3$-based systems. The selected examples highlight the impacts of the relevant microstructural features, including the presence of porosity, phase morphology and interfaces, on the thermoelectric properties and their evolution with time.

I10. Air stable triplet harvesting in nanoconfined domains of hydrogels and bioplastics

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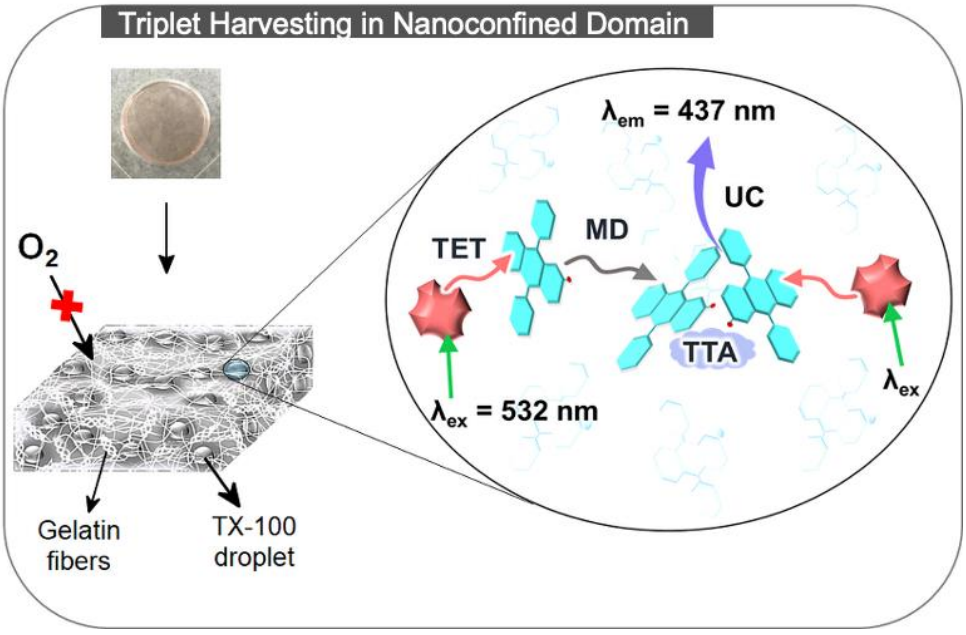
Triplet-triplet annihilation-based photon upconversion (TTA-UC) in aqueous environments and solid-state faces issues of chromophores aggregation and deactivation of excited triplets by dissolved oxygen molecules. In this talk I will present our new strategy of biopolymer surfactant-chromophore coassembly to overcome these challenges. Air-stable TTA-UC with a high upconversion efficiency of 13.5% was achieved in hydrogel coassembled from gelatin, Triton X-100 and upconverting chromophores (triplet sensitizer and emitter). The keys are two-fold. First, gelatin and the surfactant self-assemble in water to give a developed hierarchical structure with hydrophobic domains which accommodate chromophores up to high concentrations. Second, thick hydrogen-bonding networks of gelatin backbone prevent O_2 inflow to the hydrophobic interior, as evidenced by long acceptor triplet lifetime of 4.9 ms. Interestingly upon drying of this hydrogel in air resulted in phase separation of liquid TX-100 domains containing chromophores confined inside the transparent solid bioplastic film. The film showed even higher efficiency of 15.6 % in air with unprecedented durability of two years.



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I11. Optical and magnetocaloric properties of $HoCr_{0.5}Mn_{0.5}O_3$ compound

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Rare-earth orthochromites ($RECrO_3$; RE: trivalent rare-earth ion) are the vital class of functional materials having unique structural, optical and magnetic properties, which make them promising for various potential applications including thermomagnetic switches, spintronics, photocatalyst, magneto-optic and data storage devices *etc*.. We synthesized $HoCr_{0.5}Mn_{0.5}O_3$ compound and investigated its optical and magnetic properties. Rietveld and Raman analysis showed an increase in the orthorhombic distortion due to the tilting/rotation of CrO_6 octahedral. Diffuse reflectance spectroscopy confirmed a direct band gap for this compound. The photoluminescence spectrum of the present compound showed blue and green emissions at 468, 478 and 547-572 nm attributable to the transitions of $^5F_2+^3K_8 \rightarrow ^5I_8$, $^5F_3 \rightarrow ^5I_8$ and $^5F_4+^5S_2 \rightarrow ^5I_8$ levels of Ho^{3+} ion, respectively. The dc magnetization data revealed the Cr^{3+} and Ho^{3+} ion ordering temperatures ~ 66 K and ~12 K. By fitting the magnetic susceptibility data with modified Curie-Weiss law that includes Dzyaloshinskii-Moriya (DM) correction term, the strength of symmetric and antisymmetric Cr^{3+}-Cr^{3+} exchange interactions was determined. The non-zero value of antisymmetric exchange constant (D_e) affirmed the canted nature of Cr^{3+} spins due to the DM interaction. It was found that $HoCr_{0.5}Mn_{0.5}O_3$ compound exhibited an increase in the magnetic entropy change ($-\Delta S$) in comparison to that of the pristine $HoCrO_3$ compound under the same magnetic field. The magnetocaloric effect was also analyzed by Landau phenomenological theory and its results were found to be similar to those obtained using Maxwell's thermodynamic relation. The higher relative cooling power alongwith a significant $-\Delta S$ and a second-order magnetic transition makes $HoCr_{0.5}Mn_{0.5}O_3$ compound a potential candidate for magnetic refrigeration in the cryogenic temperature range.

I12. Solution blow spinning as a versatile technique for nanofibers production: an overview

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Polymeric, composite and ceramic nanofibers are extensively produced and studied for several applications. The electrospinning technique is the main processing route used to produce nanofibers around the globe, showing good reproductivity and high-quality nanofiber mats production. However, the low production rate associated with a complex experimental setup is the main drawback in its implementation on large scale. On the other side, the innovative solution blow-spinning exhibits a production rate of 3 to 10 times higher, low cost, and easy implementation. Here, we will demonstrate the principles of solution blow spinning to produce, ceramic and polymeric nanofibers. A systematic study on the influence of solution parameters (concentration, viscosity, and solvent) and experimental parameters (injection rate, air pressure, rotational speed of the collector, and size of the needle) on the formation and morphology of the fibers are demonstrated.

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I13. Crystal structure and resistive switching in NiO

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Metal oxides display a wide variety of physical properties, stimulating interest from the point of view of fundamental physics and device engineering. NiO is anti-ferromagnetic and a charge transfer insulator. However, nickel vacancies are common and give rise to an effective p-type doping. NiO sees application in spin valves, supercapacitors, hole transport layer in perovskites solar cells, water splitting (Fe doped NiO) and gas sensing.

The macroscopic properties of NiO are extremely sensitive to the presence of point defects. Cation vacancies can induce half-metallicity. In the latter, single defects can produce half-metallicity in either spin channels locally. However, the interaction of vacancies resulting in half-metallicity in the same spin channel is predicted to be energetically favourable. Nickel oxide's antiferromagentic order is predicted to persist even in the presence of the cation vacancy and resulting half-metallicity. The resistive switching observed in a NiO appears to be due to intrinsic point defects. These defects produce states at various levels within the energy gap, which are likely responsible for transport within the insulator. Therefore, study of real structure of high-quality single crystals and thin films of NiO is an important task of material science.

The (100) surface of NiO and Li doped NiO were studied after ion bombardment and annealing in UHV by photoemission spectroscopy, XRD , LEED, AFM, TEM, STEM and STM/STS. The single crystals were grown by floating zone melting. Different types of inhomogeneities in a range of mm-scale to nano-scale were observed. In particular, AFM/STM images reveal the unusual nanogranular structures on NiO(100) surface. TEM and STEM experiments demonstrate self-assembling of Ni vacancies, that resulting in creation of nanogranular structure. The nature of the observed nanogranular structure was studied using ab initio simulations. The first principles calculations showed that the possible reason of the nanogranular structure formation is the lattice distortions induced by Ni vacancy. According to the DFT calculations the diameter of the distorted area around the Ni vacancy is 1.2 nm. That is close to the size of the granules observed by SPM and TEM. The granules of NiO_x oxides are coupled coherently through common structural elements [1].

STM/STS experiments reveal temporally switching of electronic structure in a local region of the sample after a bias voltage pulse was applied at the STM probe.

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I14. Synergistic effects of $MoS_2/NiFe_2O_4$ nanocomposites for high-performance energy conversion and storage applications

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One of the great challenges in the twenty-first century is producing powerful electrochemical energy conversion and storage devices for powering several kinds of applications. The performance of these devices depends intimately on the properties of their materials. As a member of a two-dimensional materials family, molybdenum disulfide (MoS_2) has attracted great interest in recent years because of its unusual mechanical, electrical, and optical properties. On the other hand, nickel ferrite ($NiFe_2O_4$) exhibits rich redox chemistry with adequate electrical properties. Therefore, using a facile hydrothermal approach we have synthesized the $MoS_2/NiFe_2O_4$ nanocomposites (MN) and utilize the merits of each of these materials to achieve high specific capacitance and electrocatalytic performance. The symmetric supercapacitor device based on MN5 delivered a high specific capacitance of 246.68 F/g at a current density of 0.5 A/g with a high-energy density (21.92 Wh/kg) and high power density (17972.10 W/Kg). Moreover, MN5 nanocomposites catalyst exhibited a lower overpotential of 125 mV for the hydrogen evolution reaction (@ 10 mA/cm^2) and 300 mV (@50 mA/cm^2) for the oxygen evolution reaction, with excellent stability in alkaline electrolyte. This excellent electrochemical performance is accredited to the rational designing of nanocomposites, which provides more guidance for the future fabrication of high-performance electrode materials.

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I15. Re-orientation of tilted-axes graphoepitaxial fluorite films towards small-index crystallographic planes

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Re-orientation of thin films during epitaxial growth with alignment of the small-index crystallographic planes (SICPs) along the surface of the film was often observed for different materials. This effect was usually limited to very small inclination angles of the lattice and the *h,k,l* indexes of the SICPs were usually 1 or 0. We report on re-orientation of graphoepitaxial fluorite thin films towards SICPs (012), (013), with inclination angles up to 5º. Three conditions should be fulfilled for such a re-orientation: (i) the initial orientation of the film must be in vicinity of the orientation of the SICP, (ii) the film structure should show certain plasticity to allow re-orientation due to formation of defects, and (iii) the deposition conditions should promote formation of these defects.

The CeO_2 films on $NdGaO_3$ tilted-axes substrates (TAS) showed re-orientation towards (012) plane in the intermediate range of deposition rate and/or oxygen partial pressure. For lower deposition rate (higher oxygen pressure) the film grows graphoepitaxially, completely oxygenated and relaxed. For higher deposition rate or lower oxygen partial pressure the oxygen deficiency results in stronger bonds between the substrate and the film and formation of completely strained CeO_2 lattice and corresponding graphoepitaxial tilting of the film axes. In the intermediate range the plasticity of the film is high enough for defects formation, but the bonds with the substrate are insufficient to impose strict epitaxial relations, providing possibility of re-orientation of the film.

The Y:ZrO_2 films on $NdGaO_3$ TAS at standard deposition conditions always followed the graphoepitaxial growth mode. Suppressing of the epitaxial bonding between the film and the substrate by intentional depletion of substrate surface with oxygen provided necessary conditions for re-orientation of the Y:ZrO_2 film towards SICPs. The effect was observed both for (012) and (013) planes.

The re-orientation is obtained easier, reaching inclination angles of 3-5º, when the film experiences additional tilting towards the substrate plane. The re-orientation from the substrate plane is also possible, but such films are usually re-oriented partially, and the observed inclination angle is limited to 0.2-0.5º.

The re-oriented films show a lower spread of orientations of domains, revealed as a decrease of the width of the rocking curve. The reason is the orienting effect of the substrate surface during growth, opposite to the mis-orienting effect of dislocations generation for ordinary graphoepitaxial films. The lattice of the films experiences distortion of lattice due to surface tension, contractive for CeO_2 surfaces and tensile for Y:ZrO_2 surfaces. This effect is observed as an increase of the lattice constant normal to the surface plane for CeO_2 films and shrinking of the lattice constant for the Y:ZrO_2 films. With thickness of the film the tetragonal distortion increases, as revealed by an increased lattice constant variation of the re-oriented films, compared to the ordinary films.

I16. Carbon nanotubes boost cell modulation

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Carbon nanotubes (CNTs) are recognized for their outstanding mechanical, electrical, thermal, optical and structural properties. In this work, we demonstrate the use of tailored CNT micropillars templates to control orientation of cell growth.

Vertically aligned micropillared multi-walled CNTs (MWCNTs) were grown on Si/SiO_2 substrates by using lift-off lithography and chemical vapour-phase deposition. The MWCNTs micropillars were arranged as arrays, stripes and spirals in order to evaluate the MWCNTs capabilities to induce cell alignment. In addition to flat surfaces, Si/SiO_2 micropillars were fabricated by reactive ion etching to be used as control samples.

The use of CNTs to boost cell alignment was demonstrated for two distinct applications: human neurite outgrowth [1] and chondrocytes guidance [2]. In both applications, MWCNTs have supported long-term survival of the cells in comparison to the control templates. In contrast to tight bundles wrapping Si/SiO_2 pillars, single neurite interact and anchor to MWCNTs pillars forming highly organized and seamless neuronal networks. These templates enabled guidance of human neurites along any created patterns (such as spirals and stripes). Similarly, chondrocytes do align according to the MWCNTs micropatterned pillars. In this case, chondrocytes displayed an elongated morphology between the MWCNTs micropillars, with wrapping of the cell cytoskeleton around the pillars with multiple anchor points, while cells attach with thick bundles to the Si/SiO2 pillars.

Our results strongly suggest that MWCNTs properties play a bigger role than the nanotopological cue provided by the nanostructured templates. Our hypothesis is that MWCNTs based templates provide multiple cues including electrical, mechanical and chemical cues, which cannot be achieved with other materials such as Si/SiO_2 and polymer-based nanostructured templates. These templates were also transferred to microelectrode arrays to evaluate cell electrophysiology.

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I17. Nanoscale crystallization mechanisms in a GeSSbCsCl glass-ceramic and relationships with mechanical and optical properties

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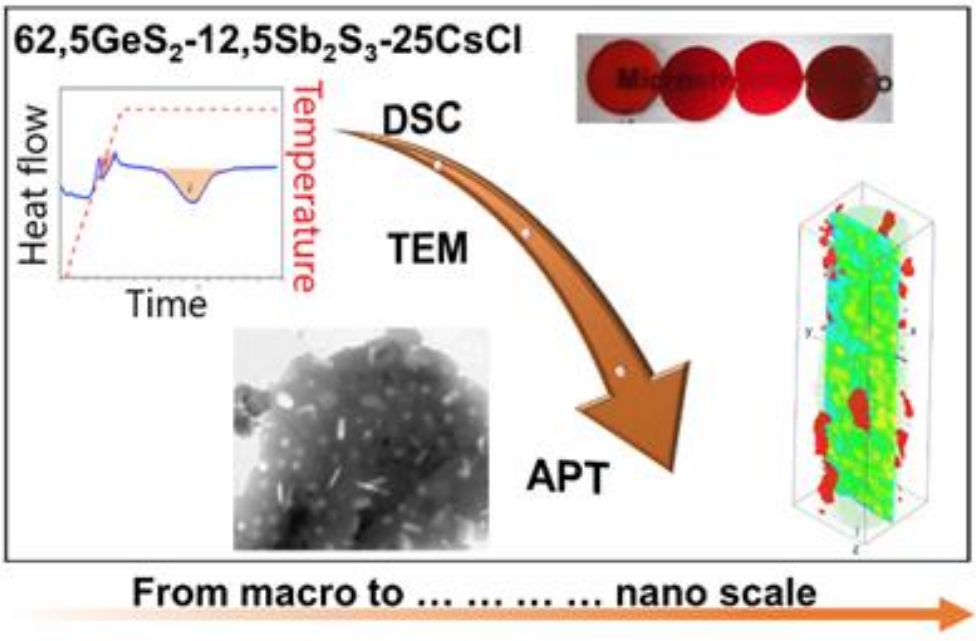
Crystallization of a 62,5GeS_2-12,5Sb_2S_3-25CsCl glass-ceramic was investigated using different techniques from macro to nano-scale: DSC (Differential Scanning Calorimetry), MT-DSC (Modulated Temperature DSC), TEM (Transmission Electron Microscopy) and APT (Atom Probe Tomography). A two-step crystallization process was evidenced, allowing a direct correlation between the microstructural features and the evolution of the mechanical and optical properties. This two-step crystallization process starts with the nucleation of spherical CsCl crystals that progressively evolve toward a disc shaped morphology when they grow. This transformation goes along with a local enrichment of Sb leading also to a significant increase of the lattice parameter of the CsCl phase. These crystals significantly improve the mechanical behavior of the glass with only a small reduction of the infrared transmission properties [1].



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I18. Insights into multiscale rotating machinery R&D: from macro to nano

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- In this talk, one of a common and important application of fluid mechanics and its interaction with solid is discussed, Rotating machinery or turbomachinery: turbines, compressors, pumps, fans… play an important role in the energy and industrial process. The scientific and the technical progress that the world knows today has all revolutionized: the size of the systems, the performance, materials and even processes. For this, the research work that take as a subject "Rotating machinery" focus mainly on their behavior dynamic to improve their performance and ensure their reliability. The mastery of dynamics of rotating machines consists in determining their resonance and their amplitude deformation so that they can avoid damage, this is often insured using the classical motion laws (classical theory of elasticity) for modeling and other techniques for simulation and optimization like: FEA and CFD.

Ongoing with the recent industrial evolution that has revolutionized the R& D in almost all fields, machines have become smaller, efficient and smarter. Thus, researchers and engineers have developed a number of nanomachines (nanomotors[1], nanorobots, nanodevices…) based on nanoscience and nanotechnology applications. In the present study, a journey through rotary small scale machines insighting into :

- Type of rotating Nano machines and their applications
- Nanomaterials, synthesis and manufacturing method
- Continuum mechanics Modeling and investigation
- Case studies

In this talk, we have reviewed the state of the art of multiscale rotating machinery, their applications, their modeling, and their features…

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I19. Emergent piezoelectric materials based on self-assembled peptides: application prospects

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Diphenylalanine (H-Phe-Phe-OH, FF) is one of the self-assembling peptides that have recently become the subject of intense research in the field of nanomaterials due to their ability to spontaneously form well-ordered structures: nano- and microtubes, nanospheres, nanofibrils and hydrogels. Peptide FF nanotubes (PNT) possess unique biological and physical properties such as biocompatibility, high rigidity, noticeable thermal stability, interesting electronic, nonlinear optical and photoluminescent properties, as well as exceptional piezoelectric effect [1] and pyroelectricity. Despite the promising prospects for self-assembling peptide systems, their practical application is still limited due to the difficulty in obtaining stable, high-performance devices.

In this work, we will discuss and analyze the emergent physicochemical [2], dielectric [3], optical and mechanical properties of peptide assemblies focusing on their understanding and further improvement based on our experience in this field.

We will compare the technological potential of their application in future devices, such as controlling the self-assembly of peptides to develop unique nanostructures for biocompatible acoustic transducers, tiny biosensors based on piezoelectric effects, energy harvesters, etc, and also discuss how modeling can help experiments to create individual functional nanostructures of peptides with controlled morphology.

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I20. $(BaCa)(ZrTi)O_3$ lead-free piezoelectrics: Recent advancements and perspectives

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Lead-free piezoelectric ceramics have emerged as a topic of intense scientific interest in the early 2000 in response to enhanced environmental awareness reinforced by impending legislation. Together with the increasing market share and improved performance of lead-free piezoelectrics, this growing realization that the use of lead should be limited in piezoelectric materials has boosted the development of lead-free piezoelectric ceramics. Lead-free candidates that are anticipated to replace highly efficient lead-based piezoelectric ceramics include alkali niobate, sodium bismuth titanate and barium titanate (BT)-based formulations.

It was not until 2009, following the work of Liu and Ren [1] that the BT-based materials modified with Ca^{2+} and Zr^{4+} caught the attention of scientific community due to the finding of outstanding electromechanical properties such as d_{33} > 500 pC/N and d^*_{33} > 1000 pm/V at 0.5 kV/mm in the compositional range between $(Ba_{0.88}Ca_{0.12})(Zr_{0.12}Ti_{0.88})O_3$ (BZT-40BCT) and $(Ba_{0.82}Ca_{0.18})(Zr_{0.08}Ti_{0.92})O_3$ (BZT-60BCT). In particular, a large piezoelectric performance with d_{33} ~620 pC/N was observed in the optimal composition $0.5Ba(Zr_{0.2}Ti_{0.8})O_3$-$0.5(Ba_{0.7}Ca_{0.3})TiO_3$ $[Ba_{0.85}Ca_{0.15})(Zr_{0.1}Ti_{0.9})O_3]$, popularly addressed as BZT-50BCT or simply BCZT. Ever since its recognition, an abundance of research work has been carried out on BCZT encompassing numerous application areas.

A summary on the recent progresses in BCZT piezoelectric ceramics achieved through chemical modifications will be presented. The potential application of BCZT ceramics/thin films including electrocaloric effect, biomechanical energy harvesting and energy storage, among others will be reviewed. In addition to the novel fields of application, insights into toxicity and biocompatibility of this family of materials will be cited as well.

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I21. Ferroelectricity in epitaxially strained rhombohedral ZrO_2 thin films

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Zirconia and hafnia based thin films have attracted considerable attention in the last decade due to their ferroelectric behavior at few nanometer scale, which can enable the downscaling and design of a next-generation functional memory devices. The present work combines experimental structural studies with DFT calculations to disclose a novel rhombohedral R3m epitaxially-strained phase of (111)-oriented ZrO_2 thin films grown by ion-beam sputtering deposition technique on (111)-Nb:$SrTiO_3$ substrates. Comprehensive local and macroscopic ferroelectric characterization reveals that these ZrO_2 films display a switchable ferroelectric polarization reaching 20.2 μC/cm^2 with a coercive field of 1.5 MV/cm. Moreover, the time dependent polarization reversal characteristics of Nb:STO/ZrO_2/Au film capacitors exhibit the typical bell-shape curves associated with domains reversal feature of ferroelectric films. The estimated activation field is comparable to the coercive field obtained from polarization-electric field hysteresis loops. Interestingly, the studied films show a ferroelectric behavior *per se*, i.e. a technological advantage over the previously studied conventional orthorhombic ZrO_2 films where it is indispensable to apply wake-up cycles to induce ferroelectricity.

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I22. Antiferrodistortive phase transition in doped strontium titanate ceramics: a role of the perovskite lattice vacancies

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$SrTiO_3$-based compounds have been attracting considerable interest both from a fundamental point of view and for a wide range of applications [1]. Fundamentally, perovskite-structured $SrTiO_3$ undergoes a cubic (Pm3m) to tetragonal (I4/mcm) phase transition at ~108 K (T_a) associated with rotations of the O octahedra in antiphase around the [001] direction. This phase transition gives rise to modes at the R-point of the Brillouin zone. Here, inelastic light scattering is used to study the lattice dynamics of $SrTiO_3$ ceramics with isovalent and heterovalent dopants, substituting for Sr^{2+} or Ti^{4+} ions [2-5]. Even for a small percentage of any of the dopants, T_a is significantly altered, varying oppositely to the tolerance factor (t) [2,3]. In the case of Sr-site donor dopants (La^{3+}, Gd^{3+}, Y^{3+}), a common linear dependence of T_a versus t is obtained, if strontium vacancies with a size ~7% larger than Sr^{2+} radius are taken into account [4,5]. On the other hand, Ti-site substitution with acceptor Mg^{2+} dopant or sintering $SrTi_{0.95}Mn_{0.05}O_{3-\delta}$ ceramics in N_2 suppress T_a due to a creation of oxygen vacancies, disrupting the octahedra connectivity needed for their cooperative rotation [2].

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I23. Nanoscale imaging of functional properties of perovskite solar cell using atomic force microscopy

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In 2009 a group of Tsutomu Miyasaka published a seminal article [1] demonstrating a new class of photoabsorption materials for solar cells – hybrid organic inorganic perovskites (HOIP). In one decade photoconversion efficiency (PCE) increased from 3.8 % to more than 25 % on a single HOIP solar cell and surpassed 29 % on perovskite/Si tandem solar cells [2]. HOIPs are defect tolerant and can be prepared by low temperature solution processing, thus enabling low-cost perovskite solar cells. Their band gap and optoelectronic properties are easily tuned in a wide range by simple halide substitution [3], which make HOIPs attractive for photovoltaic application beyond solar cells, e.g. LEDs, photodetectors, etc. The main remaining challenge hindering HOIPs applications is operational degradation.

Continuous progress in intrinsic stabilization of the perovskite layer [4] and optimization of the device architecture and interfaces [5] substantially increased the long term stability of perovskite solar cells, however it is still far from >20 years lifetime of conventional Si solar cell modules. Here we report on implementation of Atomic Force Microscopy for investigation of fresh and degraded under operation conditions perovskites, including in-situ measurements. The obtained data include topography and functional properties such as local surface potential and local photocurrent. Combined with macroscopic methods such as current-voltage characterization, XRD, UV-Vis and PL spectroscopy, it allows deeper understanding of degradation mechanisms.

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I24. Mechanisms of nucleation, growth, and stabilization of local ferroelectric states in organic piezoelectrics

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Organic polar materials have emerged as critical electro-active materials [1]. During the last decade, many studies have been focused on their polar nature [2]. The origin of dipole moment in organic piezoelectrics is often associated with hydrogen bond displacement/rotation [1,2] or collective electron/proton transfer [1,2]. Charge-transfer and intramolecular charge transfer compounds appear to be a promising class that reveals distinctive piezo- and ferroelectric properties at room temperature [2,3]. In this work, we have studied the piezo- and ferroelectric behavior of such compounds (DPFO microfibers, glycine aminoacid microcrystal, peptide microtubes) by atomic force microscopy (AFM) in the piezoresponse mode, supplemented by micro-Raman spectroscopy at room temperature and above. The obtained results reveal possible mechanisms responsible for the origin of piezo- and ferroelectric D–π–A domains, where the effect of cooperative structural rearrangements was observed to be dependent on the sample thickness.

The reported study was funded by RFBR according to the research project № 20-02-00422.

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I25. Rare earth doped thermographic phosphors for non-contact temperature sensing

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Sensing temperature in various environments would be a very difficult process, as they may be physically harsh / chemically hazardous / corrosive or biologically vulnerable. But the need to sense the temperature is indubitable. A non-contact way of determining the temperature would be more beneficial for those types of environments. Different phosphor materials possess different unusual properties to withstand these harsh environments.

The presentation describes different approaches in sensing temperature via non-contact approach using photoluminescence that could be possible with RE doped nanomaterials. Luminescence thermometry based on time integrated such as spectral shifts, change in bandwidths, intensities, shapes, and polarizations as well as based on time-resolved such as emission decay times and rise times would be explicitly presented with specific examples.

As part of presentation RE doped nano/micro sized materials with upconversion / down conversion / down shifting capabilities would be presented. Exclusive results of materials such as RE^{3+} doped REOF, $SrGd_2O_4$ and several oxide ceramics will be presented with their relative sensitivities and methods.

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I26. $CrNb_3S_6$ single crystals grown by gas transport method

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Layered structure of some semiconductors, such as NbS_2, provides a possibility of intercalation of metal atoms between the matrix layers. This results in producing T_xNbS_2 ternary compounds (where T = Mn, Fe, Co, Ni), which can possess ferromagnetic properties, provided that they have a certain stoichiometric composition and an ordered lattice.

In this work we consider Cr_xNbS_2 (x= 1/3), which is known for it ferromagnetic properties below the transition point. The main obstacle in growing these crystals is instability of their composition. Most often a mixture of two phases is obtained with x=1/3 and x=1/4, which are both ordered phases, and some disordered solution may also present in a solid state.

There were three main purposes: to grow single crystals with ordered lattice, to study their phase and chemical composition, to measure most precisely Curie temperature.

To do so, two-stage gas transport growth using I_2 as an agent was designed. To analyze chemical composition of the product of the reaction EPMA method was used. To study phase composition XRD Rietveld analysis was used, and the structure was tested by a Gemini-R X-ray diffractometer. Field and temperature dependencies of high frequency (HF) absorption in a $CrNb_3S_6$ single crystal were measured in periodically swept magnetic field to obtain Curie temperature.

As a result, single crystalline plates of 3-5 mm and about 0.5 mm thick were grown at the second stage of the reaction. Their almost completely ordered $CrNb_3S_6$ superlattice with [0001] orientation has the unit cell parameters a = 5.744Å, c = 12.132Å, which is in good correlation with our XRD data: a = 5.737Å, c = 12.124Å.

The final compound was produced from the initial synthesized powder, which consisted of $CrNb_3S_6$ and Cr_6S_7 microparticles transformed at the first stage into a mixture of $CrNb_3S_6$ and $CrNb_4S_8$ and Nb and Cr iodides, which then oxidized and evaporated.

Temperature dependence of HF absorption in parallel and normal to the sample periodic magnetic field was measured to estimate Curie temperature of the $CrNb_3S_6$ single crystal. Ferromagnetic ordering of the sample was detected below 115 K.

I27. Facile strategies for nanoconfinement of magnesium hydride for hydrogen storage

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Currently magnesium hydride is the only reversible hydride (capacity: 7.6 wt.% H_2) that reaches the capacity target (5.5 wt.%) for the light duty hydrogen fuel cell vehicles [1,2]. However, the significant issue is that the experimentally observed H-desorption temperature of MgH_2 (>350 °C) is far higher than the temperature target, 85 °C. This is because of the high H-desorption enthalpy change (ΔH = 75 kJ/mol) and high activation energy (Ea = 149 kJ/mol) of MgH_2. Recent works prove that both the ΔH and Ea values can be lowered appreciably by restricting the particle size of MgH_2. It is possible to reduce the size down to nano order by top down approaches, however, due to the higher tendency of agglomeration of Mg/MgH_2 particles it is difficult to maintain the size when we recycle the samples. In order to address this issue, nanoconfinement strategies were adopted in the current study. We have initially reduced the size of MgH_2 particles by ball milling treatment for 30h (size: 20-60 nm) and then impregnated the particles on the pores/grooves of activated charcoal (AC) scaffold using a programmed heat treatment at 550 °C under 5 bar pure hydrogen ambient. The result obtained by this approach is found to be better and more consistent than the materials prepared by melt infiltration at 650 °C or vacuum heated samples under 550 °C. Especially, the activation energy value (88 kJ/mol) obtained in the case of impregnated catalyst free material is far better than the activation energy value of the unconfined material (149 kJ/mol). In another strategy, we have also identified that instead of confining MgH_2 on the pores of AC, additives can also be loaded on the pores and in this case only a very small amount of nanoconfined additive (typically 3 wt.%) is sufficient for improving the performance of MgH_2 by over 10 orders of magnitude.

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I28. YAG:Ag nanophosphors – synthesis and characterization

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Research and development of nanophosphors is a part of rapidly growing nanoscience and nanotechnology. Yttrium aluminium garnet (YAG) – based phosphors have attracted significant interest owing to their excellent luminescence characteristics. In the present work, YAG and the Ag doped YAG (0.5, 1.0, 1.5 and 2.0 mol% of Ag) was prepared by Pechini method. The synthesised YAG is white in colour but the incorporation of Ag in the YAG matrix forms colour centre and turns to pink colour. $Y_3Al_5O_{12}$ yttrium aluminium garnet nano particle and Ag doped YAG was prepared by Pechini method. The pure phase of YAG and Cubic structure was confirmed from the XRD pattern and indexed as per the JCPDS data. The sharp peak in the XRD reveals the good crystalline nature of the samples. Lattice expansion is indicated by the shift of XRD peaks towards lower diffraction angle after the Ag incorporation. The bending and stretching vibrations of the oxygen groups associated with YAG was observed in FTIR spectra. Tube like morphology was noticed in the SEM and increase in crystallite size is also perceived after the incorporation of Ag in YAG matrix. The melting of grain suggested that the sintering temperature is high. The elemental mapping confirmed the purity of synthesized samples and it is in accordance with the calculated values. The optical absorption and luminescent characteristics of the sample was analyzed using UV-Vis and Photoluminescence spectra.

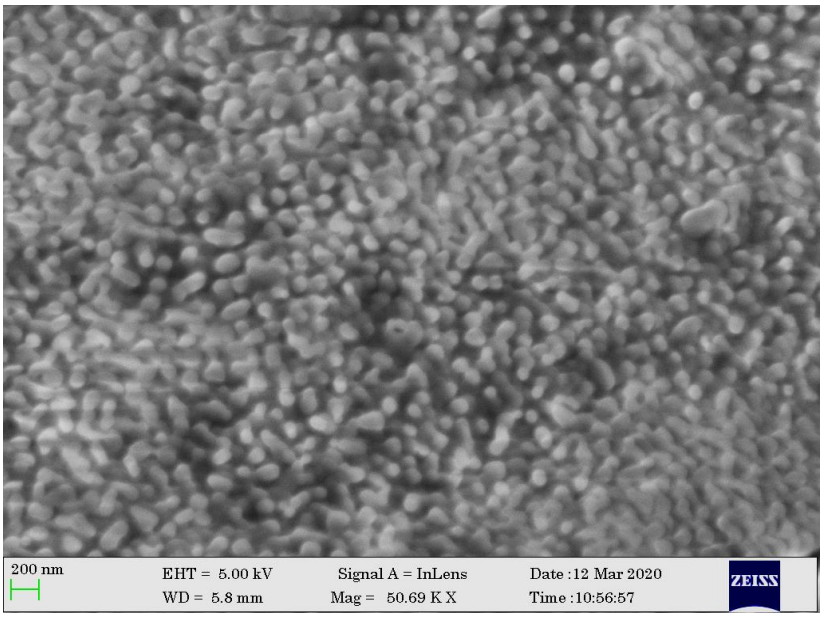

Figure 1. Scanning electron micrograph of Ag(0.5 wt%) doped YAG

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I29. Raman study of ammonia thermal diffusion in diphenylalanine nanotubes

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Self-assembled peptide nanotubes can serve as channels for the transportation of water and other small molecules with high diffusion coefficients [1]. This work presents a study of the diffusion of ammonia molecules (NH_3) in diphenylalanine nanotubes (FF NTs) under the action of a temperature gradient. Variations of NH_3 local concentration in the nanochannels studied *in situ* directly by confocal Raman microscopy yield an estimate of the ammonia thermal diffusion coefficient $D = 5.9\times10^{-12}$ m^2s^{-1}. Due to the strong adhesion of NH_3 molecules to FF walls, the temperature gradient leads to an inhomogeneous density of molecules, which, in turn, results in the appearance of a pressure difference and the movement of molecules from a denser (cold) region to a less dense (hot) one. Additionally, the thermal conductivity coefficient $\lambda \approx 3.78\times10^{-4}$ W m^{-1} K^{-1} estimated for the first time for FF NTs is comparable with that of keratin nanofibres (4.62×10^{-4} W m^{-1} K^{-1} [2]).

This work was developed within the scope of project CICECO-Aveiro Institute of Materials (UIDB/50011/2020 & UIDP/50011/2020) and the project UniRCell (SAICTPAC/ 0032/2015, POCI-01-0145-FEEDER-016422) financed by national funds through the FCT − Fundação para a Ciência e a Tecnologia, I.P. (Portugal). S.K., P.Z., and A.K. were supported by FCT through the project “BioPiezo”- PTDC/CTM−CTM/31679/2017 (CENTRO-01-0145-FEDER-031679) and F.M.L.F. by the project UniRCell. P.Z. and V.Y. thank Russian Science Foundation (grant No. 18-72-0052). The equipment of the Ural Center for Shared Use “Modern nanotechnology” UrFU was used.

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Oral presentations

O1. Magnetic field, heat transfer and rheological analysis of a magnetorheometer using finite element method

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Magnetorheological (MR) fluids show changes in apparent viscosity under an applied magnetic field. As a result, dramatic and reversible changes in rheological properties occurred, which permits many electromechanical devices to have potential utility in the aerospace, automobile, medical, and another field. Therefore, there is a need to investigate the rheological properties and heat developed due to changes in rheological properties of MR fluids under the uniform magnetic field. This work presents the numerical simulation of magnetostatic, laminar fluid flow, and thermal field distribution of a plate-plate magnetorheometer using the finite element method. We analyzed the magnetic field distribution and magnitude of the magnetic field along the radius of the plates. We obtained a better uniform magnetic field along the radius of the plate with enhanced the magnitude of the magnetic field at a particular applied current compared to the other existing design of the rheometer. The maximum magnetic flux density at 4A of coil current is 1.3T. Laminar flow simulation gives the shear stress at the applied magnetic field as a function of shear rate. We obtained the maximum velocity of the magnetic particles at the outer radius between plates. The heat generated due to the electromagnetic coil and slippage heating between the plates (i.e., MR region) is 302.5K and 308.5K at 3A current after 40 minutes of working. The maximum temperature generated due to the combined effect of the electromagnetic coil and slippage is about 318K after 40 minutes of working, much below the operating temperature of MR fluids. Here we enhanced the magnetic field density profile and magnitude of magnetic flux density along the working radius of the plate and minimized the effects of resistive coil heating in the MR fluid region by the coil and location design.

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O2. The efficient solar-light-driven photocatalytic performance of hybrid reduced graphene oxide/TiO_2/graphitic carbon nitride composites for organic pollutant degradation

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Accelerated industrial development in recent years has a negative influence on the aquatic ecosystem. Pollutants such as pesticides, microplastics, persistent organic pollutants, and dyes are present. In several industries, including cosmetics, plastic, paper, textiles, and rubber, synthetic dyes are used to give color to the products. The massive scale of used synthetic dyes, which are chemically and thermally stable in water, represents a potential hazard to the environment. The photocatalytic removal/degradation and wastewater treatment under solar-like irradiation have their own limitations. It is necessary to solve major challenges to overcome the drawbacks of the conventional water treatment processes.

In this research, the hybridized photocatalyst was successfully synthesized as a mixture of pure TiO_2 particles, reduced graphene oxide (rGO), and graphitic carbon nitride (*g*-C_3N_4). The graphene oxide (GO) material was synthesized by Hummer's method using natural graphite flakes (particle size ≤ 50 μm). The bulk *g*-C_3N_4 was prepared by a simple pyrolysis procedure using urea as a precursor. The hybridised rGO/TiO_2/*g*-C_3N_4 photocatalyst has been self-assembled through one-pot hydrothermally synthesis followed by an annealing treatment. The morphological and structural analysis of the fabricated photocatalysts have been analyzed by X-ray diffraction (XRD), Fourier transforms infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). Photocatalytic experiments with solar-like irradiation were performed to evaluate the efficiency of the synthesized materials. Composites were used as photocatalysts in the degradation of dye Methylene blue (MB) dye in an aqueous medium at a pH of 5.9. In addition to the natural pH of the solution (5.9), four other pH values (3.3, 7.3, 10.5, and 12.5) were adjusted and the efficiency of MB degradation was studied.

The synthesized rGO/TiO_2/*g*-C_3N_4 hybrid shows higher photocatalytic activity than pure TiO_2 particles, TiO_2/rGO, and TiO_2/*g*-C_3N_4 composites in the degradation of MB dye in an aqueous medium (10 mg/L) under solar-like irradiation. The obtained results show that the photocatalytic activity of TiO_2 increases with a higher amount of added rGO and *g*-C_3N_4. The pH of the solution also affects the MB degradation rate. Therefore, the high-efficient hybridised rGO/TiO_2/*g*-C_3N_4 photocatalyst could have the potential for environmental remediation.

O3. Micro-Electrical Discharge Machining (µEDM): Effect of physical and electrical parameters on crater size

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The growing market for Microsystems (MST) and Micro-Electromechanical Systems (MEMS) is driving the research for alternative manufacturing techniques to microelectronics-based technologies, which are generally expensive and time-consuming. Hot-embossing and micro-injection modeling of thermoplastics appear to be industrially viable processes [1]. However, both require the use of master models, usually made in hard materials such as steel. These master models cannot be fabricated using standard microelectronics processes [2]. Thus, other micromachining processes are used, as laser machining or micro-electrical discharge machining (µEDM) … In this work, we are interested in µEDM.

The principle of µEDM is based on the use of a cylindrical thin tool that erodes the workpiece surface. The two electrodes are immersed in a dielectric with a distance of a few micrometers (gap) [3]. When an electrical potential is applied between the two electrodes, electrical discharges are generated which cause material erosion.

In order to produce master models with high resolution and smooth surfaces, it is necessary to well control the discharge mechanism. However, several problems are encountered, such as a random electrical discharge process, the fluctuation of the discharge energy (fig.1). Thus, a better control of the erosion requires an in-depth study of the effect of the different parameters (applied voltage, working capacity, gap…).

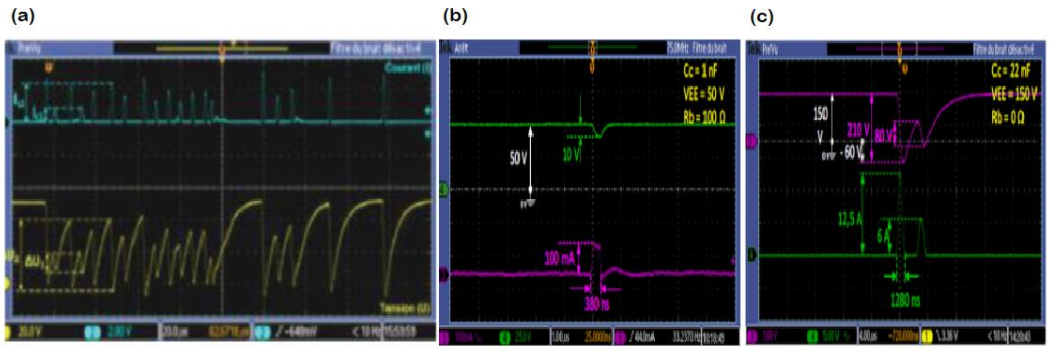

Figure 1. Discharges obtained with the Lazarenko generator, (a) example of discharges, (b) without reverse polarity, (c) with reverse polarity

In this article, we present the experimental results obtained to characterize the effect of different parameters: Electrical polarization (workpiece/electrode), machining voltage, working capacity, micro-tool diameter, gap, …

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O4. Aerodynamic efficiency analysis of winglet using CFD

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The winglets are a means to increase the effective wing aspect ratio without increasing structural loads. the objective of the use of winglets is to improve the wing fuel efficiency and decrease the vortex behind the wing. a computational analysis of wing without winglet and with winglet attached to the wingtip was studied by the commercial code ANSYS FLUENT 14.0 to establish the aerodynamic performance by designing two winglet configurations for different angle of attack. the first design is the blended winglet with cant angles of 60° and a new winglet design was performed and compared to the basic blended winglets. the new design was a group of three blended winglet with different cant angles: 60°, 65° and 70°. the flow was fully turbulent for free stream velocity of 50 m/s and the turbulence model used is Spallart Allmaras. the results showed that the bended winglet increase the lift to drag ratio i.e. aerodynamic efficiency by reducing the drag and the vortices behind wing. Furthermore, the blended winglet group decreased the lift to drag ratio, however the blended winglet group are able to reduce the vorticity therefore reduced the induced drag.

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O5. Conjugated poly(metalla-yne)s for new materials applications

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Conjugated poly(metalla-yne)s (Fig. 1) constitute an important class of fascinating materials in view of their potential applications in opto-electronic (O-E) devices such as photo-cells, field-effect transistors (FETs), photo switches, light emitting diodes (LEDs), liquid crystal displays (LCDs) and non-linear optics (NLOs) [1]. In poly(metalla-ynes) the photo-physical properties of transition metal fragments are coupled to those of the organic poly-ynes. For example, the incorporation of heavy metal fragment like bis(trialkylphpsohine)Pt(II) along the polymer backbone introduces large spin-orbit coupling to allow light emission from the triplet exited state. In this context, Pt(II) poly-ynes incorporating a wide variety of spacer groups have been widely investigated in our laboratory. Pt-poly-ynes are excellent triplet emitters. The triplet states in Pt-poly-yne can be investigated through, by direct optical excitation. Consequently, the Pt-poly-yne can serve as model compounds to study the basic photo-physical properties of conjugated hydrocarbons poly-ynes. The conjugated spacer is important in tuning the O-E properties of the Pt(II) poly-ynes. The incorporation of a second metal such as Re(I) as a pendant side-chain into a Pt(II) poly-yne was found also to affect the photophysical properties of the obtained materials [2,3]. Herein, we present the experimental and theoretical studies of some Pt(II) poly-ynes and explore their potential for application in O-E devices.

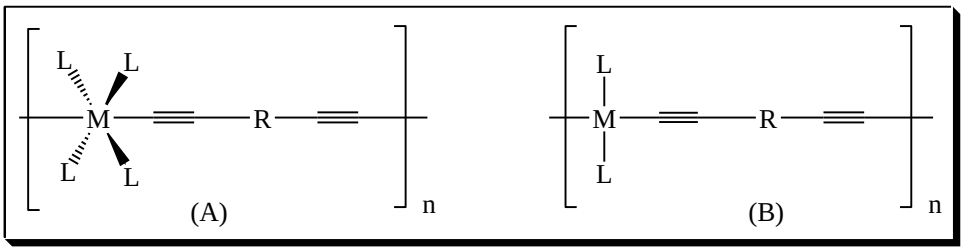

Fig. 1. General chemical formula of poly(metalla-yne) backbone.

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O6. Electromechanical characterization of chitosan-based films

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Chitosan is the second most abundant polysaccharide in the world. It is obtained from the deacetylation of chitin, which is the main structure in the shell of different mollusks and insects. This biopolymer has been recognized as an excellent material for wound healing and preservation applications due to its non-toxic and antibacterial properties. In recent decades chitosan has been studied for other applications such as biomedical sensors and actuators as it presents electrical response to mechanical stimulus [1], but the results are not conclusive so far [2], [3]. In this work, solvent cast films containing 1.5% w/v of chitosan dissolved in acetic or lactic acidic media were prepared with 0, 25 or 50% of glycerol plasticizer. The structural analysis suggests that the addition of glycerol affects the semicrystallinity of the films. The mechanical characteristics indicate that the films fabricated with lactic acid are ~16% more elastic and stretchable than those with acetic acid, and these properties increase by ~93% with the addition of glycerol in both cases. The presence of the plasticizer also improves the thermal stability of the films. The piezoelectric sensitivity increases by 50% for the films fabricated with acetic acid. These results indicate that there is a strong correlation between the physical-mechanical properties and the piezoelectric sensitivity of the films.

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O7. Fluorescent nanomaterials-based optical sensors for detection of environmental contaminants

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All over the world, environmental pollutants and their associated hazards are of major concern. Therefore, the quantification of theses pollutants or contaminants (like heavy metals, pesticides, etc.) in water or food has gained significant research interest. In comparison to conventional laboratory-based approaches for quantification of these contaminants, the research efforts have been directed towards the novel sensing techniques keeping in view high sensitivity/selectivity, ease of operation, throughput readouts, and simple setup. Among these sensing techniques, optical biosensors have significant potential to satisfy the requirements of cost-effective and rapid quantitative detection. In optical biosensors, fluorophores interact with analyte that causes subsequent changes in intensity of their fluorescence which can be correlated to the quantity of the analyte. With advancements in material science, the fluorescent nanomaterials are replacing the conventional fluorophores due to their superior optical properties such as high photostability, option of selection of excitation and emission wavelengths, excellent fluorescence, etc. The optical characteristics of nanomaterials can be controlled through their size or shape that facilitate the selection of diverse fluorescent probes for high throughput. Present work deals with quantification of these pollutants via different fluorescent nanostructures as sensing probes. Here, we have synthesized different nanostructures involving metal-organic frameworks (MOFs), quantum dots (QDs), and their composites. The formation of these nanostructures and further functionality is confirmed by different spectroscopic and microscopic techniques. The potential of these nanostructures is explored for detection of heavy metal ions in water samples.

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O8. New way of conceiving the structure of graphene

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The author proposes to divide the bonds in molecules into *bi-electronic* (with the participation of two electrons = covalent) and *mono-electronic* (with the participation of one electron = non-covalent). The result of the commonality of a single electron in a bond is the formation of a bipolar orbital, generating a force of attraction. Moreover, in the proposed model, the formation of tetrahedral, planar and linear molecules is not caused by the presence of three types of orbital hybridization (sp3, sp2, sp), because the mechanism of creating different bonds does not consist in changing the conformational geometry of individual atoms (hybridization), but in changing the relationship spatial dimensions between atoms that cause changes in bond lengths (predictable by trigonometric equations), angles between atoms and the topology of molecules. Carbon atoms transforming from cyclohexane to benzene to achieve charge saturation do not undergo hybridization, but form multiple bonds, transforming the *bi-electronic* bonds into *mono-electronic* bonds and changing the spatial relationships of the atoms so that the available electrons approach the dipole orbitals, as shown in the figure. This makes it possible in benzene to use only one electron for each bond, making two electrons statistically available for each carbon to form the crosslinking of the pi bonds above, below, outside and inside the ring. This tight cross-linking of pi bonds gives benzene and graphene exceptional structural stability and exceptional properties. Moreover this new model of benzene is able to explain different characteristics of this compound and its derivatives without resorting to resonance theory, for example the differentiation of spin density of adjacent hydrogens in the ring, differentiation between the activating and deactivating substituents of electrophilic substitutions, degrees of aromaticity of the condensed rings and the annulenes. Graphene is the multiplication of the benzene fuel structure, therefore the determination of the exact structure of benzene is the first step in the knowledge of graphene.

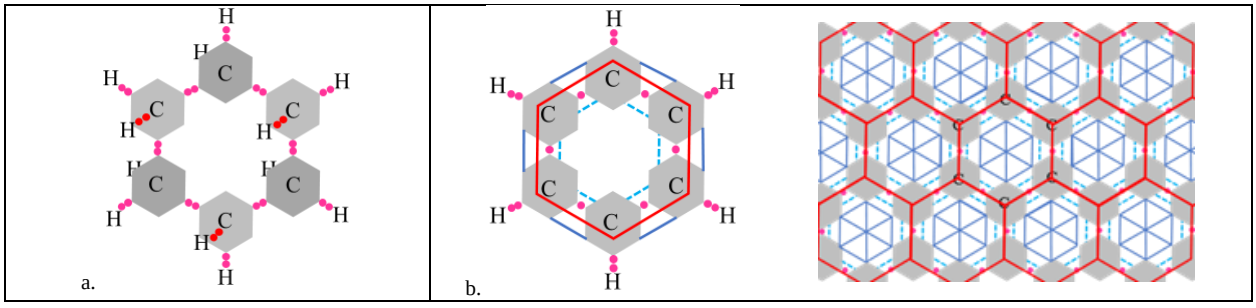

Fig. 1. Colors indicate binding plans and single line indicates an electron of the π bond equally shared between two atoms. a) Cyclohexane: bond length C - C ≈ (√3l) / 2 ≈ 153.20 pm, bond angles ≈ 109.5°. b) Benzene and graphene: bond angles ≈ 120°, bond length ≈ (√2l) / (√3) ≈ 141.98 pm but the C-C bond in benzene is stretched only in two directions which reduces its calculated value.

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O9. Nanoparticle-infused-biodegradable-microneedle technology for skin cancer treatment

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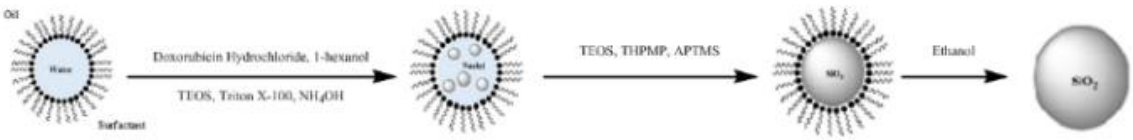

Figure 1 - Schematic diagram of the microemulsion method used for synthesis of anti-cancer drug-doped nanoparticles

Melanoma affects over 200,000 people in the UK alone, with survival rates of around 86%. Over the last decade melanoma skin cancer incidence rates for males and females combined increased by 50%. The current main treatments of skin-cancer are surgery to remove the affected area, as well as chemotherapy/radiotherapy and immunotherapy to kill the tumour cells. However, around 33,000 people still die within the first five years after diagnosis and treatment. The purpose of this study is to explore the possible development of a new nanomedicine technology that uses anti-cancer drug doped-nanoparticles to kill tumour cells. For almost two decades, scientists were exploring the use of nanoparticles as drug vesicles capable of protecting their cargo and deliver it to the target site while evading detection by the body. However, their translation to clinical use has been slower than expected. To a large degree, this is due to the difficulty to formulate the nanomaterial into a usable form, in which they retain their unique, size-dependent properties without aggregating into a bulk material. The proposed solution to this is to formulate the nanoparticles into a microneedle array made from carboxymethyl cellulose gels. Carboxymethyl cellulose is used specifically because it is biodegradable and will degrade by enzymatic reaction in the epidermis, thus releasing nanoparticles into the microenvironment. Microneedle patches have been used widely in cosmetics[1], as well as for insulin delivery[2]. In this work, we describe a simple methodology for synthesising novel biodegradable microneedle[3] systems infused with silica nanoparticles[4] (SiNP). SiNP were doped with a small library of model anti-cancer drugs or drug surrogates before being characterised and encapsulated into biodegradable microneedles. Detailed preparation and characterisation methods for both the nanoparticles (figure 1) and the microneedles-infused with nanoparticles (figure 2) is presented here. We demonstrated the distribution of the nanoparticles within the microneedle matrix in a uniform, un-aggregated form, which enabled the release of the nanoparticles in a sustained manner. To observe the disintegration of microneedles and the release of the drug-doped nanoparticles in the skin[5], optical coherence tomography (OCT) has been used[6] (figures 3 & 4). Although OCT has been used widely in ophthalmology, the use of OCT to image the skin is still relatively new[7]. Formulating nanomaterial into biodegradable, hydrogel-

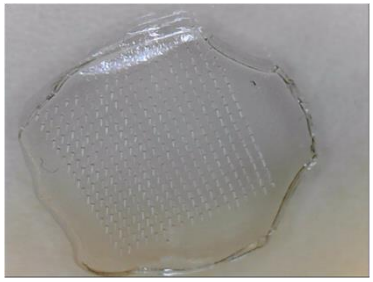

Figure 2 - Microneedle array structure consisting of 324 needles of height 750 µm, base diameter 200 µm, tip diameter 10 µm and centre-to-centre spacing of 600 µm

like microneedles showed to be effective in preserving their colloidal properties, whilst simultaneously enabling the transdermal delivery of the nanomaterial into the body. Although the concepts of nanoparticles and biodegradable microneedles have been researched individually, the combination of the two, to the best of our knowledge, offers a new pathway to nanomedicine-related applications.

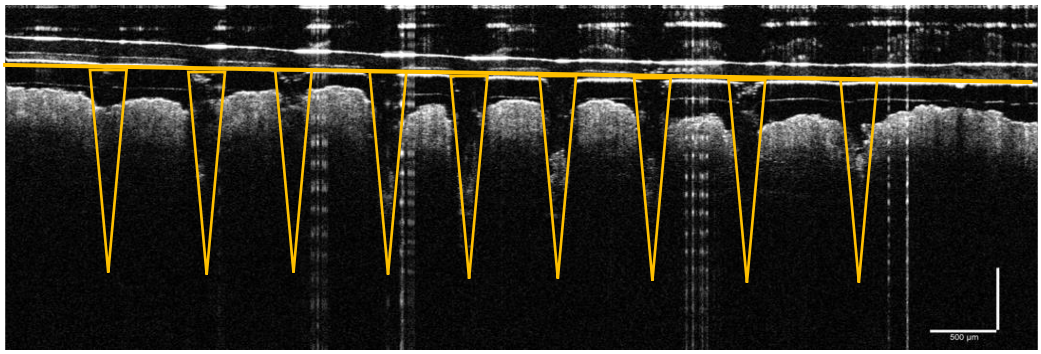

Figure 3 - B-Scan OCT image of microneedle array in skin - microneedle shape highlighted by yellow

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O10. Structural and physical properties of Sr-substituted hydroxyapatite: modeling and experiments

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Hydroxyapatite (HAP) is widely used as biocompatible materials for a variety of medical applications. It is known that some substitutions in HAP cation and anion sublattices can improve the mechanical properties of HAP ceramics and influence the activity of osteoblasts and osteoclasts, that facilitate more rapid implantation of such modified HAP ceramics. Efforts are made for improving the HAP properties for this aim, particularly, via substitution of strontium ions for calcium ions.

Structural and physical properties of Sr-substituted hydroxyapatite (HAP) - with substitution of strontium for calcium atoms (Sr/Ca substitutions) are considered and analyzed in this work. Modeling and calculations of the HAP properties values that change due to Sr/Ca substitution are proceeded by the methods of density functional theory (DFT) in various approximations [1–3]. The available experimental data [4-6] are analyzed in comparison with these calculation results.

1) Calculation data of structural changes (lattice constants and cell volume) at Sr/Ca substitutions in HAP for different calculation methods used and their comparison with experimental data [4] showed that there are obvious similar changes - an increase in all these parameters after Sr/Ca substitution.
2) Changes in mechanical and elastic properties were studied - calculated values of the bulk modulus and other elastic characteristics calculated before and after Sr/Ca-substitution was analyzed in their correspondence to the observed data.
3) Changes in optical properties were studied (band gap Eg, spectral properties) - an increase in the calculated band gap Eg was noted after Sr/Ca-substitution. Corresponding increasing in the electron work function $\Delta\phi$ were established also in these calculations as a result of the Sr/Ca substitution, (especially noticeable in combination with vacancy of the OH group [1]).

It should be noted, that earlier, in a number of experiments, it was shown that an increase $\Delta\phi$ leads to an increase in adhesion and proliferation of bone cells [5]. Moreover, as it was shown the doping of HAP with Sr atoms also increased the adherence of bone cells to the HAP surface [5, 6].

Thus, the increase in the work function $\Delta\phi$ obtained in our calculations for Sr/Ca substitutions in HAP corresponds to the experimentally observed data on an increase in

the number of osteo-cells (osteoblasts, osteoclasts) and their higher growth (proliferation) on HAP Sr-substituted surfaces [1, 5, 6].

The positive correlation obtained according to our density functional modeling and calculations indicates the importance of Sr/Ca substitution for improving the biocompatibility and quality of implant based on the modified HAP, containing Sr/Ca substitutions.

The study was supported by a grant Russian Science Foundation (RSF) - project No. 21-12-00251.

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O11. Two-step sintering of alumina with the addition of waste alumina powder

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The impact of the two-step sintering (TSS) process on the obtained microstructure of alumina ceramics with and without the addition of waste alumina powder was studied. Alumina samples were formed according to the slip casting method by preparing alumina suspensions with commercial alumina powder (99.9 mass%-Al_2O_3 content, 0.8 μm average particle size). The second set of alumina suspensions was prepared by mixing up to 20 dwb.% (expressed on a dry weight basis) of waste alumina powder with commercial alumina. The waste alumina powder (99.7 mass%-Al_2O_3 content, 3.4 μm average particle size) was collected after the green machining step in the industrial manufacturing process of alumina ceramics. Except for alumina powders, dispersant Tiron (0.05 dwb.%), binder Polyvinyl alcohol (0.1 dwb.%), sintering additive Magnesium Aluminum Spinel (0.2 dwb.%) were used to prepare stable alumina suspensions. After sintering ceramic green bodies, morphological analyses were performed. The intercept method was applied to determine the average grain size from the obtained SEM images, while sample porosity was calculated based on apparent densities. Furthermore, a comparison of the mechanical properties of alumina samples lacking and containing 20 dwb% of waste alumina powder obtained by TSS is presented. The indentation fracture toughness and Vickers hardness slightly increased compared to alumina samples lacking waste alumina powder. The better mechanical properties of ceramic samples containing waste alumina are a consequence of lower porosity. The reported results suggest the possibility of recycling waste alumina powder in a ceramic material.

O12. Formation of ohmic contacts to the thick films on the basis of Bi_2Te_3 solid solution prepared by screen printing

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The development and formation of devices operating on the basis of thermoelectric phenomena is currently an actively developing field of science and technology. One of the promising areas is the conversion of human-generated thermal energy into electricity using flexible thermoelectric generators (TEG) integrated into clothing and wearable electronics.

The method of screen printing with using suspension is one of the promising and cheap methods for creating flexible TEGs, which allows the formation of legs of random size. However, the thermoelectric legs formed by this way have a number of disadvantages, such as: an undeveloped technology for creating legs by this method and creating ohmic contacts to them, as well as high resistance and low Seebeck coefficient in comparison with polycrystalline thermoelectric material. In this regard, the purpose of this work was development of method for forming thermoelement legs by screen-printing and ohmic contacts to them.

To form the legs of the n- and p-type thermoelements, the powder of the thermoelectric material was mixed with a binder, after which experimental samples were formed by screen-printing through a metal mask. An aqueous alkaline sodium silicate solution was used as a binder. The formation of an electric contact to the legs was carried out by two methods: by pressing in a copper wire and by the method of electrochemical deposition; Cu and Ni were used as the deposited metals.

The results showed that the formed contacts are ohmic, and the samples with electrical contacts formed by the electrochemical deposition method have a lower resistivity by almost an order of magnitude than the samples with a wire contact. Investigations of the temperature dependences of resistivity were carried out, as well as an investigation of the Seebeck coefficient. The results obtained showed that the use of this technology is promising for the manufacture of flexible thermoelectric generators.

O13. Investigation of the crystallization kinetics for thin film of phase change memory material on the basis of $GeSb_2Te_4$

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For the last few years electrical phase change memory has attracted more and more attention in the field of non-volatile memory devices. For the formation of phase change memory cells, materials of the Ge-Sb-Te ternary system are used most widely [1]. $GeSb_2Te_4$ (GST124) is considered to be promising material for the technology of phase change memory. However, the crystallization process in GST124 thin films, which determines operation speed of phase change memory cells, is poorly understood [2].

In this regard, the purpose of this work was to study the features of the crystallization kinetics for thin films of the $GeSb_2Te_4$ material.

GST124 thin films were formed on silicon wafers by magnetron sputtering of a GST124 target. The thickness of the obtained films was 1.5 μm. The composition was studied by Auger spectroscopy and energy dispersive X-ray spectroscopy. Structural features were determined using X-ray diffraction. Thermal properties, phase transition temperatures, and crystallization kinetics were investigated by differential scanning calorimetry (DSC). The measurements were carried out in aluminum crucibles at 5 different heating rates in a nitrogen flow on a DSC-50 calorimeter.

Three phase transitions were found on the obtained DSC curves, which correlates with the literature data. In the temperature range 158-169 °C, a crystallization peak is observed. The transition from the metastable cubic phase to the stable hexagonal phase is present in the temperature range 259-299 °C. The temperature of the onset of the melting peak at 603 °C was also determined. An endothermic peak appeared in the temperature range of 400-425 °C after the second measurements of the sample, which is due to the melting of the eutectic in the Ge-Te system. Obtained parameters allowed to analyze the crystallization kinetics of GST124 thin films.

This work was supported by a grant from the President of the Russian Federation (MK-5457.2021.4).

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O14. MXene-containing composite electrodes for hydrogen evolution

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MXenes are shown to be promising electrocatalysts either alone or as a part of the MXene-based materials [1]. Ni-based electrodes are commonly used as cathodes in alkaline electrolysers for the production of hydrogen, provided by their low cost and corrosion resistance [2, 3]. This work explores the possibilities for the processing of Ni- and $Ti_3C_2T_x$ (T = OH, O) MXene- containing composite electrodes for hydrogen production. In order to tune the Ti_3C_2 interlayer distance in Ti_3C_2Al MAX phase, an introduction of additional Al to form $Ti_3C_2Al_z$ materials with z>1 was attempted. Self-propagation high-temperature synthesis of powder mixtures with extra Ni and Al content (e.g. Ni:Ti:Al:C = 1:2:3:1) resulted in SHS products containing $Ti_3C_2Al_z$ z>1 material and Ni-Al alloys. Further etching of these products in 10M NaOH allowed the direct formation of electrodes with active surface containing $Ti_3C_2T_x$ (T = OH, O) MXene- and Raney nickel-containing composites. The electrochemical studies were focused on hydrogen evolution and showed the potential for boosting the electrochemical reaction in Ni and MXene-containing composite electrodes. The guidelines for the processing of such electrodes under fluorine-free conditions are proposed and discussed.

As a result, it was shown that the composites containing sintered Ni-Al alloys, MAX phase and $Ti_3C_2Al_z$ phase, z>1 can be obtained using the SHS process of mixtures based on Ni, Ti, Al, C powders with moderate excess of Al (e.g. Ni:Ti:Al:C = 1:2:3:1). The possibility of Al etching from such SHS products in alkaline conditions, followed by the formation of MXenes, was demonstrated and attributed to larger interlayer distance and lower diffusion limitations in the space between Ti_3C_2 layers. Partial alkaline etching of the electrodes prepared directly by SHS of Ni-containing precursors (e.g. Ni:Ti:Al:C = 1:2:3:1) allows the formation of nano-Ni/$Ti_3C_2(OH)_x$ MXene composites with notable electrocatalytic activity. An enhanced catalytic activity of nano-Ni/$Ti_3C_2(OH)_x$ MXene composite towards the hydrogen evolution reaction at higher potentials likely can be attributed to the acceleration of the Volmer stage in HER process, by enhancing the water adsorption and dissociation on the catalyst surface.

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O15. Bacteria capture with magnetic nanoparticles modified with cationic carbosilane dendritic systems

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Magnetic nanoparticles (MNP) have shown great potential in different fields (environmental, biomedical, clinical), as consequence to their many unique properties. Engineered MNP with polycationic systems are able to remove bacteria from polluted medium with high yield and short times, due to the ability of these systems to interact with the bacteria membrane [1]. One type of these systems are cationic carbosilane dendrimers, which are macromolecules that exhibit bactericide properties if they present an adequate hydrophobic/hydrophilic balance [2].

In this work, we have grafted cationic carbosilane dendritic systems on the surface of iron oxide MNP and studied their capacity to remove different pathogenic bacteria from water (*E. coli* as Gram-negative and *S. aureus* as Gram-positive bacteria) by electrostatic interaction and magnet capture. The modified MNP were characterized by transmission electron microscopy (TEM), thermogravimetric analysis (TGA), Fourier-transform infrared spectroscopy (FT-IR), Z potential and dynamic light scattering (DLS). TEM and scanning electron microscopy (SEM) also showed the interactions between our magnetic nanoparticles and bacteria.

Higher capture efficiency was achieved for MNP modified with cationic carbosilane dendrons than with cationic carbosilane dendrimers. This behaviour is explained due to the lower functionalization obtained with cationic carbosilane dendrimers, meaning lower availability of cationic groups on the surface of MNP. We have also studied different ratios MNP/bacteria and recyclability the MNP.

The results obtained make MNP functionalized with cationic carbosilane dendrons a very attractive system to be used in different applications, as could be purification of polluted water or development of new diagnostic treatments.

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O16. Zinc based metal-organic framework derived zinc-blende nanoparticles for supercapacitor applications

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ABSTRACT

The increased industrialization and demand for renewable energy have inspired the research community to improve energy storage systems. From the last decade, the rise of the Metal-Organic Framework (MOF) has been proven to a revolutionary material for various applications. Herein, we have utilized ZIF-8 MOF to derive the ZnS nanoparticles through hydrothermal synthesis methods for energy storage applications. The obtained ZnS from ZIF-8 exhibit high crystallinity, high reaction sites, and nanoparticles confirmed from various characterization techniques including XRD, FESEM, and EDS. Further, the electrochemical testing has been done in the three electrochemical systems with 1M Na_2SO_4 electrolyte solution. The ZnS nanoparticles showed a capacitance of 51.2 F/g which can be attributed to the high surface area of the nanoparticles and redox activity. Additionally, the full symmetric solid-state supercapacitor device has been assembled with 1M Na2SO4 PVA electrolyte gel. The electrochemical device showed excellent electrochemical performance with long-term cyclability.

1. INTRODUCTION

The limited supply of non-renewable sources and their adverse effect on the environment has inspired the research community to find alternatives. Batteries are the best alternatives to fulfill the demand of the futuristic technologies, however, the low power density of these devices limit its application in numerous field [1]. The supercapacitor is another class of devices works on adsorption-desorption or redox activity, has much higher power density, and thus can be combined with batteries for high performance [3]. The advancement in the supercapacitor is in its initial phase and activated carbon is the only commercialized material used for supercapacitor electrode [3]. To improve the supercapacitor performance in terms of high redox activity and high adsorption-desorption, we have derived nanoparticles of zinc-blende (ZnS) from highly porous ZIF-8 MOF. The sample showed 51.2 F/g of specific capacitance at 3A/g of current density attributed to the nanosized crystallites and high surface area of ZnS.

2. MATERIALS AND METHODOLOGY

Zinc acetate and 2-methylimidazole have been used for synthesis. The ZnS nanoparticles have been synthesized through the hydrothermal reaction of ZIF-8 in the presence of thiourea. The optimization has been done at different hydrothermal temperatures. The sample this coded as Z-n, where n is the reaction time. For the preparation of the working electrode, the active Z-24 material was mixed with polyvinylidene fluoride (PVDF) binder and carbon black in a w/w ratio of 8:1:1 to form a uniform slurry and then coated over a graffoil sheet.

3. RESULTS

The obtained three samples (Z-6, Z-12, and Z-24) have been initially characterized with XRD and FESEM for optimization purposes. In XRD, the complete formation of ZnS from ZIF-8 can be observed after the synthesis time of 24hr. The same can be observed in the FESEM images in which the ZIF-8 crystals can be seen for Z-6 and Z-12 samples. But the sample Z-24 was found to be free from any large crystal and only nanosized particles can be observed which confirms the successful formation of ZnS after 24hr.

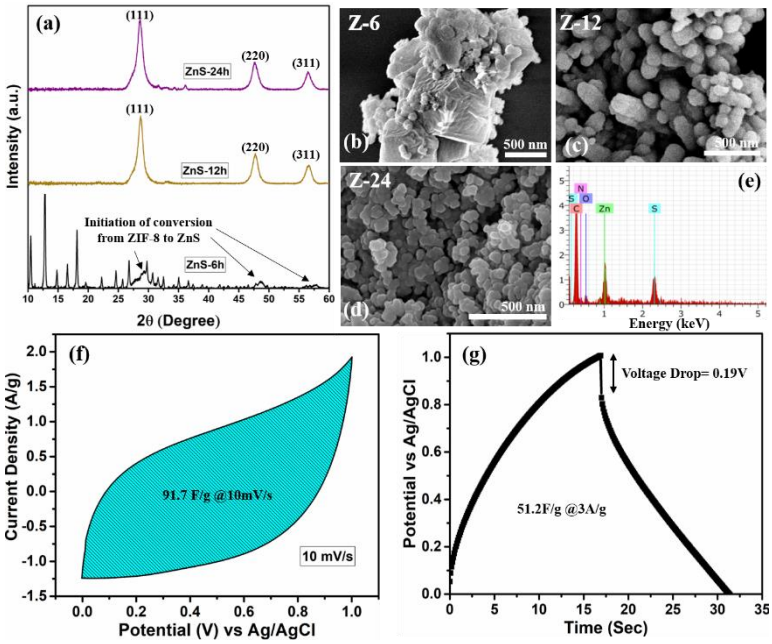

Figure 1 (a) XRD, FESEM of (b) Z-6, (c) Z-12, (c) Z-24, (d) EDS of Z-24, (f) CV, and (g) GCD of Z-24.

The Zn-24 sample was further used to investigate the electrochemical performance through cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) curve in 1 M Na_2SO_4 (Fig 1c). With CV, the specific capacitance was found to be 91.7 F/g at 10mV/s whereas, with GCD, the specific capacitance was found to be 51.2 F/g at the current density of 3 A/g.

4. CONCLUSION

The ZnS nanoparticles were synthesized from the hydrothermal route from the ZIF-8 precursor at different synthesis periods. The XRD, FESEM, and EDS test confirms the successful formation of ZnS nanoparticles with high crystallinity. Further, upon doing electrochemical characterization, the sample delivered 91.7 F/g of specific capacitance at the scan rate of 10 mV/s. The current work can further be extended to derive the conducting ZnS nanoparticles embedded in carbon structure from ZIF-8 MOF through the pyrolysis route. The strategy can be extended to other MOFs to obtain the nanoparticles of oxides and sulfides.

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O17. Synthesis of high luminescent and stable hybrid metal-organic frameworks and perovskite nanocomposite as phosphor for green LED

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Metal halide perovskites are used for various energy devices due to their excellent properties like tunable band width, ambipolar semiconducting behavior, superior electrical conductivity, etc. However, several challenges in front of them like propensity towards degradation in presence of moisture, UV radiations, etc. This work focuses on nanocomposites of perovskites and MOFs where MOFs work as a supporting template to hold the perovskite nano-crystals. MOFs are the highest porous material with high specific surface area along with good stability. Here, we synthesized MAPbBr3 and CsPbBr3 perovskite and Pb MOF-based nanocomposites by directly incorporating the perovskite precursors in the pre-synthesized Pb-MOF matrix. The synthesized nanocomposites are further characterized by different microscopy and spectroscopy techniques and the results shows high green luminescence at 520nm when excited with 360 nm wavelength which does not decreases in different RH values and shows stability for months. Further this composite was Used as a phosphor for the fabrication of green LED by coating it over blue colored UV LED. Thus, this work offers an innovative solution to improve the stability of perovskite materials for photovoltaic.

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O18. Solvothermal synthesis of MIL-125(Ti) metal organic framework and investigating its photocatalytic activity under visible light in presence of H_2O_2

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Metal–organic frameworks (MOFs) are a class of porous crystalline materials. Due to their high specific surface area, rich topology and easy pore tunability, MOFs have recently attracted increasing attention for photocatalysis. Their catalytic activity has been investigated for applications like CO_2 reduction, H_2 evolution, and organic pollutants degradation. Dye have been thoroughly used in the textile industry for the fabric colouring. They are inexpensive, changes the fabric chemically and stays permanently. But at the same time their disposal is an issue. Photocatalytic dye degradation studies have been reported with TiO_2 but only in the UV region. In regard to this, a Titanium Metal Organic Framework have been synthesized. MIL-125(Ti) is a three-dimensional porous solid composed of infinite $Ti(OBu)_4$ octahedra connected by bis-bidentate terephthalate ligands. Because of the small size of the Ti (IV)−oxide cluster, there occurs limited recombination of the photo-generated charge carriers and thus a superior photoactivities could be expected in such MOFs. MIL-125 was synthesized by using a simple one-pot solvothermal method using titanium-n-butoxide (metal) and 2-NH_2-1,4-BDC (linker) as precursor molecules and characterized by varied techniques such as Electron Microscopy, X-ray Diffraction and Spectroscopy. Lastly, it was subjected to study the photocatalytic degradation of Fluorescein Dye, with the aid of H_2O_2 and 200W LED light and exhibited a degradation of 74% after 2hrs of reaction. Additionally, the MIL-125(Ti) demonstrated excellent reusability and stability. Thus, application of MIL-125(Ti) can be a potential approach to construct an efficient heterojunction for visible light induced photodegradation.

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O19. Polyurethane/ZnS:Mn blended thin film for piezo-luminescence sensing

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Mechano-luminescent/Piezo-luminescent self trigger devices are the next level smart devices for the civil, automobile, defence and aerospace industries[1][2][3]. ZnS:Mn is one of the brightest material that has been researched well for its property of being mechanoluminescenc in nature. Present work focuses on the fabrication and testing of Piezo-luminescent thin films for self powdered optical devices. In this research, first ZnS:Mn material is synthesized using solid state reaction technique. The synthesized micro particles process blended with Polyurethane, which is optically transparent polymer. The composite slurry so formed is casted over the Lucite glass disc using a spin coating method. These casted discs then subjected to mechanical impact under a dynamic pulse pressure generator tower. The mechanical impact pressure range is kept from 40 to 400bar pressure. The optical signal so obtained with every impact is recorded with spectrometer and photodiodes. The obtained results reflects that blended composite of Polyurethane/ZnS:Mn coated disc has capacity to be used as a sensing matrix material for self triggered optical impact sensors in advanced applications.

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O20. Ferroelectric polymer based neuromorphic device

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A neuromorphic computing that mimics human brain functionalities has been considered that can overcome the limitation of von Neumann-based computing systems with its characteristics of parallel computing capability with energy-efficient data processing. From an energy efficiency point of view at the neuromorphic system, many candidates for synaptic devices have been suggested such as phase-change memory, resistive change memory, conductive bridge memory, and ferroelectric memory. However, it is still challenging to implement low power neuromorphic system with these emerging memories since more switching power reduction should be realized for parallel array application. Among the aforementioned applications, the ferroelectric device is one of the promising candidates for synaptic devices due to its low power and fast switching characteristics.In this work, we investigated the ferroelectric synaptic device based on ferroelectric field effect transistor (FeFET) structure using polyvinylidenefluoride-trifluoroethylene (P(VDF-TrFE)) copolymer. We fabricated FeFETs with respect to various PVDF weight percents, PVDF / TrFE composition ratio, and thickness of the ferroelectric polymer. Each sample's ferroelectric characteristics e.g. coercive field, remnant polarization, and hysteresis were evaluated. Additionally, the synaptic plasticity characteristics such as long-term potentiation and long-term depression (LTP/LTD), and spike-timing-dependent plasticity (STDP) were thoroughly examined with each FeFETs. With these efforts, we could analyze the relation between ferroelectric switching properties and synaptic plasticity characteristics.

O21. A study on the streak patterns of the spin coating process

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The spin coating process is the method to make a thin film having a uniform thickness. In the semiconductor industry, the spin coating is mostly conducted for the photo-resist coating to be used as masking film during the photolithography process. It proceeds as a wafer is placed on the rotating chuck and then the photo-resist is deposited on the center area of the wafer and the photo-resist spreads out to the edge side of the wafer and forms a thin film. It is important to understand the impact of each control factor on the thickness and uniformity of the photo-resist to achieve predictable and reproducible photo-resist thickness. In this paper, we investigated the thickness variation phenomenon with respect to the viscosity of the photo-resist on each wafer position using computational fluid dynamics simulation. In addition, we conducted experiments on the real wafers reflecting the simulation results and evaluating the optimum condition to reduce the thickness variation.

O22. Fabrication and microstructure optimization of highly porous $BaZr_{0.85}Y_{0.15}O_3$ ion-conducting ceramics

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Manufacturing of solid oxide cells for NO_x decomposition in exhaust gases requires good chemical compatibility of electrolyte with Ba-containing electrocatalysts, such as $La_{2-x}Ba_xNiO_4$ ceramics. $BaZr_{0.85}Y_{0.15}O_3$ electrolyte has good compatibility with Ba-containing compositions and a sufficiently high level of oxygen ionic conductivity. Integration of solid oxide cells into the systems with the flux of exhaust gases requires the manufacturing of highly porous cell components to reduce backpressure and overcome gas diffusion limitations. The current work is focused on the manufacturing of porous $BaZr_{0.85}Y_{0.15}O_3$ ceramics employing paraffin micelles as a pore former. The Taguchi experimental planning was applied to find the optimum composition of suspension/emulsion while reducing the number of routine experiments. The task was to establish the correlations between the content of each emulsion component (paraffin, surfactant, and binder) and parameters of fabricated ceramics: porosity, gas permeation, microstructure, and pore size distribution.

The prepared porous $BaZr_{0.85}Y_{0.15}O_3$ ceramics showed high open porosity (virtually no closed pores) while preserving a sufficient level of mechanical strength after sintering at 1500°C. Morphology was quantified by GrainSizeTools/ImageJ software. Average cell size and distribution can be adjusted by emulsion composition in a wide range: from several to tens of microns. Total porosity varies in the range of 70-75%, with the level of intergranular porosity of around 20%. The sodium dodecyl sulfate surfactant content has the highest effect on pore size distribution, while the paraffin content determines the total level of porosity. The distribution nature was found to be close to log-normal by frequency. In the case of excessive surfactant/binder content, the distribution can be bimodal due to foaming or competition of breakup and coalescence during stirring. It was found that $BaZr_{0.85}Y_{0.15}O_3$ ceramics slowly reacts with water in suspension with the formation of $BaCO_3$, leading to an increase in pH up to 13. However, this does not affect the emulsification process, the decomposition is reversible, and sintered porous ceramic is single-phase.

O23. Prospects of metallurgical waste valorisation by the electroreduction of $Fe_{2.3}Mg_{0.7}O_4$ ceramics to Fe

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The alkaline electrochemical reduction of iron oxides arises as carbon-lean alternative technology for steelmaking, with lower electric energy consumption [1]. Moreover, the valorisation of metallurgical waste with high iron content represents an interesting approach for decreasing the over-exploitation of natural resources such as iron ores. In this scope, the present work consists on the electrochemical reduction of a magnesium ferrospinel material into iron under strong alkaline conditions, for studying the prospects of using a metallurgical waste as an iron oxide source. Porous ceramic samples of $Fe_{2.3}Mg_{0.7}O_4$ were processed based in the ceramic suspensions of powders with water, followed by the emulsification of liquid paraffin to create highly-porous cellular structures as in [2]. The electrochemical reduction tests were performed both in bulk ceramic samples and in powder suspensions after crushing the ceramic pieces in the latter case. All electrochemical tests occurred at 90 °C, at strong alkaline conditions (10 M, NaOH), where Ni grids were used as substrate. A Pt wire was used as counter electrode (CE) and a Hg|HgO|NaOH (1 M) electrode as a reference electrode (RE). Cyclic-voltammetry curves, chronoamperometry curve performed at potentiostatic mode (-1.14 V, 6 h) and electrochemical impedance spectroscopy (EIS) were recorded by a VersaSTAT 4 (AMETEK) potentiostat. Combined studies of XRD/SEM/EDS proved the presence of Fe crystals in both electrochemical systems. Despite a magnesium hydroxide phase was also observed in both cases, blocking the progression of the electroreduction, a 55% of Faradaic efficiency was attained in the bulk system. The magnesium phase showed to have a significative impact during the electroreduction in the suspension mode, lowering the efficiency to 20%. Nevertheless, the electroreduction to Fe was proved in both systems and the reduction mechanisms were studied. Low content of magnesium impurities can be considered for the valorisation of metallurgical waste by the electroreduction technology.

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O24. Finite element method analysis of two carbon fiber reinforced polymer propellant tanks using different manufacturing methods

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Mass reduction is of paramount importance in the design of space launch vehicles (SLV), where the inert weight has a major impact on the performance. The main propellant tanks are the main contributors to the dry mass of an SLV [1], wherefore it is of great interest the manufacture of these components in composite materials, which offer both superior specific resistance and rigidity. In spite of the application of these materials facing several challenges in the past, leading to aluminum-copper-lithium alloys being the state-of-the-art [1], recent advances are allowing the use of carbon fiber reinforced polymer (CFRP) materials in this application [1]. Our previous work has shown that a mass reduction of at least 35% is possible through the use of CFRP compared to metallic materials [1]. Thus, the purpose of this work is to analyze two CFRP main propellant tanks using the finite element method (FEM), one modeled with particularities of the fiber winding manufacturing process, whilst the other is modeled with cloth and tape lay-up. Both tanks have the same overall volume and dimensions, and the boundary conditions include the maximum flight loads to which the related SLV is subjected. This analysis offers the possibility of assess the impact of each manufacturing method on the structural strength of the propellant tanks, which, in turn, allows a greater understanding of how the composite materials behave in the structure of a main propellant tank. Furthermore, an additional decrease in mass has been achieved over the previous work [1].

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O25. A luminescent DPA@Zn-MOF composite for plausible applicability in light emitting devices

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Luminescent Metal Organic Frameworks (MOFs) on account of their augmented fluorescence lifetimes, quantum efficiencies, and large scale tunability could be highly useful in future light emitting devices. Composites of luminescent MOFs with electroluminescent complexes as emissive materials could result in display devices with outstanding emission efficiencies. In the present work, a stable blue emitting DPA (Diphenyl anthracene) @Zn-MOF novel composite has been synthesized and tested for opto-electronic behavior. Inheriting dual characteristics of high luminescence, emission lifetime, stability, tunability of MOF as well as low band gap, thermal stability, electroluminescence of the CBP complex the synthesized composite material exhibited highly promising behavior in regard to potential applicability in light emitting devices.

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O26. *Nostoc sp.* immobilized rGO-PPy nanocomposite based photoanode for bio electricity generation in non-mediated bio photovoltaic cell

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There is utmost requirement of exploration of suitable electrode nanomaterial having excellent conductivity, high specific surface area, good biocompatibility, and chemical stability for potential application in Bio-photovoltaic devices. Novel or modified 2D electrode nanomaterial with inherent conductive properties may enable fabrication of high-performance bio photovoltaic cells in context of net power output. The applicability of graphene and its nanocomposite with conductive polymer in BPVs offers promising results than conventional ITO and carbon based electrode materials due to enhanced conductivity and high surface area which also enables effective adsorption of cyanobacteria, exhibiting augmented power production and durability. Therefore, the present work focuses on the synthesis of an efficient rGO-PPy nanocomposite based photoanode for bio electricity production using a cyanobacterium called *Nostoc sp.* (NOS) in bio photovoltaic cell. The immobilization of *Nostoc sp.* (NOS) on synthesized photoanode material with high electrochemical activity and stability facilitates enhanced power output in electrochemical fuel cell set up which further lays foundation for construction of cost-efficient and high-performance BPVs.

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O27. 2-D nanomaterials-based biosensor for aflatoxin detection

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Aflatoxins are hepatotoxic secondary metabolites which are highly carcinogenic and adversely affects human health. They are produced by Aspergillus *flavous* and Aspergillus *parasiticus.* These fungal species are resistant to food treatment methods such as cooking, heating, sterilization etc. resulting their high levels in food products and making them primary health hazard. So, there is a need to develop a sensitive and reliable method for the detection of traces of aflatoxins in different food products. The detection methods should be sensitive and specific due to the low concentration of aflatoxins in different food products. In the present work, 2-D (MoS_2) nanosheets were synthesised by hydrothermal method and used for the electrochemical detection of aflatoxins. The synthesised nanosheets were characterised using various structural and morphological techniques (XRD, SEM, FTIR). Further, MoS_2 nanosheets were electropolymerized on screen printed carbon electrode (SPCE) and then anti-Aflatoxin (AFB1) antibodies were attached over the modified SPCE electrode. The different concentrations of aflatoxins (AFB1) were prepared and incubated with MoS_2 nanosheets modified electrode. These electrodes were further used for the detection using various electrochemical techniques such as cyclic voltammetry electrochemical impedance spectroscopy. (CV, EIS). The results shows high specificity and sensitivity towards the aflatoxins.

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O28. Water pollution control & hydrogen production using 2D- photocatalyst: 6, 13- pentacenequinone (PQ)

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Of late, inorganic material based photocatalysis helps to treat industrial waste water up to some extent. Aromatic, complex, organic dyes and pigments are the wastes which damages the human health as well as aquatic life. Researchers are working to overcome this serious issue from many years, but to developed cost-effective and eco-friendly method is unsolved challenge.

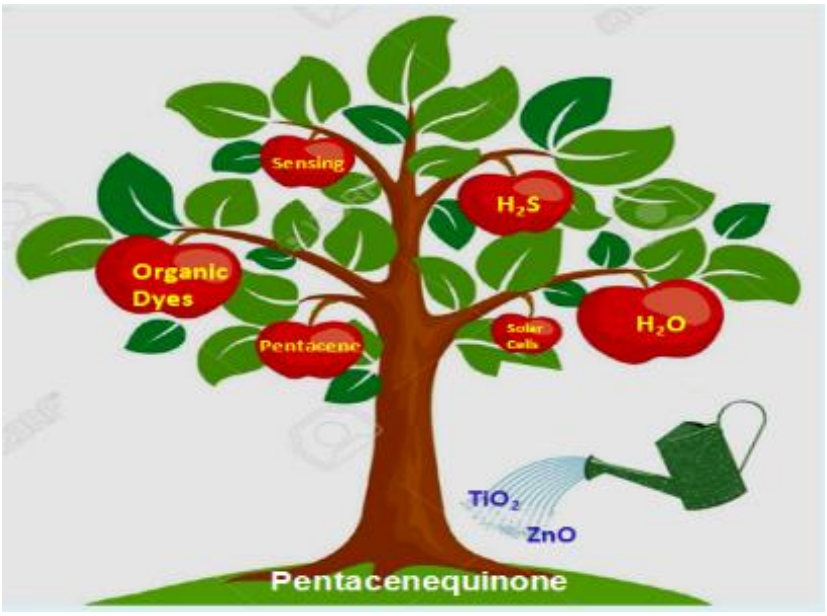

Fig. 1. Applications of 6, 13- pentacenequinone (PQ)

We have synthesized 6, 13- pentacenequinone (PQ) an intermediate require synthesizing pentacene which is well known organic semiconductor. After complete characterization we explored PQ for industrial dye degradation and photocatalytic H_2S splitting for the first time. We also synthesized composite system of PQ-TiO_2 with inorganic semiconductor photocatalyst. Recently a report of PQ-MoS_2 photocatalyst also covers the water splitting area. This organic PQ photocatalyst have high potential in photocatalysis field which can be utilized for the clean environment and for water treatment.

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O29. Iron electrowinning under alkaline conditions: effects of the current interruptions

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Nowadays, despite the rising demand of light materials, iron, namely steel, plays a crucial role in the modern world. For the time being, the main conclusion is that there are no economically feasible steelmaking technologies available that have the potential to meet the EU's climate and energy targets for 2030. At best, a 15% decrease in the overall CO2 intensity of the sector could be achieved throughout the widespread dissemination of technologies that could reasonably become cost-effective in the future. Therefore, breakthrough technologies are urgent and indispensable. An electrochemically based route is being already developed as a candidate for an alternative to conventional steelmaking processes for CO2-free iron production. Direct electrochemical reduction of iron oxides has been gaining attention as a process allowing in-situ reductions at the cathode, under strong alkaline media.

To find the feasibility of operation with long term interruptions (e.g. to seek preferential operation in low tariff periods), the experiments were performed with step changes in current rather than in potential. The selected experimental conditions comprise cycles with shut down interruptions, and other cycles with an impinged residual current (10%) to ensure cathodic protection. It seems that microstructural changes are the prevailing effect of interruption without cathodic protection in these ranges of potential/current density. Coarser grain sizes observed for unprotected shutdown interruptions may be related to surface re-structuring of the top layer, by re-oxidation during the unprotected interruption and subsequent reduction. Investigation of the cross-sections of the deposits in both regimes doesn't reveal any layer structure. The only deposit where layers were observed was obtained in the regime, where the cathodic protection step lasted 8 times longer than the deposition.

O30. Co-crystal synthesis, characterization and antimycobacterial study of cocrystals of oleanolic acid with isoniazid

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Organic cocrystal is crystal engineering that is gaining interest across different discipline. The work presented here involves investigation of co-crystals involving isoniazid(INH), a foremost first-line drug TB drug recommended for use by the World Health Organisation in the treatment of tuberculosis and oleanolic acid(OA), a hepatotoxicity naturally occurring compound and possess moderately antimycobacterial activity. The cocrystal between the two compounds was carried out for the first time using solvent evaporation, solvent drop and direct grinding methods. The co-crystal compound was further characterized using PXRD, TGA and SEM which and consequently evaluated for *in vitro* anti-TB and cytotoxicity using Human Embryonic Kidney (HEK 293) and Human Hepatocellular carcinoma (HepG2) cells. The P-XRD of the synthesized compound maintained crystalline nature like isoniazid for the three methods, while the TGA for all the three methods have cleavage values from 220^{o}c -360^{o}c, and the SEM images obtained from the three synthetic methods appears rod-like in nature. The co-crystal of OA and INH increased the anti-TB MIC values for the three synthetic methods used as follows (a) Solvent evaporation (1.06μM); (b) Solvent drop (0.50 μM); (c) Direct grinding (0.61 μM). The cytotoxicity tests of the co-crystals on the two human cell lines (HEK 293 and HepG2) were found to be IC_{50} ≥300ug/ml. The conclusion on the current research is that the co-crystal between the compounds are possible, more work is to be done on the ADME profile and it can be deploy in the treatment of HIV/TB co-infection.

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O31. Co-crystal synthesis, characterization, antimycobacterial and cytotoxicity study of cocrystals of betulinic acid with isoniazid

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Organic cocrystal is crystal engineering that is gaining interest across different discipline. The work presented here involves investigation of co-crystals involving isoniazid(INH), a foremost first-line drug TB drug recommended for use by the World Health Organisation in the treatment of tuberculosis and betulinic acid(BA), another interesting pentacyclic triterepenes just like oleanolic acid has a hepatotoxicity activity but structurally different and naturally occurring compound with moderately antimycobacterial activity also. The cocrystal between the two compounds was carried out for the first time using solvent evaporation, solvent drop and direct grinding methods. The co-crystal compound were further characterized using PXRD, TGA and SEM which and consequently evaluated for *in vitro* anti-TB and cytotoxicity using Human Embryonic Kidney (HEK 293) and Human Hepatocellular carcinoma (HepG2) cells. The P-XRD of the synthesized compound maintained crystalline nature like isoniazid for the three methods, while the TGA for all the three methods have cleavage values from 220^{o}c -360^{o}c, and the SEM images obtained from the three synthetic methods appears rod-like in nature. The co-crystal of BA and INH increased the anti-TB MIC values for the three synthetic methods used as follows (a) Solvent evaporation (0.56μM); (b) Solvent drop (0.51 μM); (c) Direct grinding (0.45 μM). The cytotoxicity tests of the co-crystals on the two human cell lines (HEK 293 and HepG2) were found to be IC_{50} ≥300ug/ml. The conclusion on the current research is that the co-crystal between the compounds are possible, more work is to be done on the ADME profile and it seems that co-crystal between INH/BA showed better activity than INH/OA and can therefore be deploy in the treatment of TB infection.

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O32. The role of long-range electrostatic interactions and local topology of the hydrogen bond network in the wettability of fully and partially wetted single and multilayer graphene

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The wetting properties of graphene and other 2D materials is a new rising field due to its wide technological repercussions, such as desalination membranes, sensors, and coating. Recently, both experimental and theoretical studies have contributed to deepening our understanding of this important field, but basic questions remain unanswered. In particular, the role of separate interactions driving wetting properties remains an intricate puzzle, and the organization of water molecules in the proximity of the surfaces, unexplored.

In this talk we present a computational method for the estimation of interfacial energies and wetting properties of water/graphitic interfaces with a special focus on fully and partially wetted (i.e., in contact with water on one side and vacuum on the other) single and multilayer graphene. Through the calculation of the local stress tensor based on the Irving-Kirkwood-Noll theory we rationalize the role of van der Waals and electrostatic interactions in the wettability. While van der Waals interactions dominate in the partially wetted system (in agreement with previous results), we have found that the wettability of fully wetted graphene is a balance between van der Waals and electrostatic interactions. In both cases we relate the strength of such interactions with the modification of the hydrogen bond network, coordination defects and diffusion in the proximity of the surface. We then propose a set of valuable tools to investigate the effect of long-range electrostatic and dispersive contributions on the wetting phenomena and their effects on the local structure. The investigation of the wettability of graphene and graphite is an important aspect in predicting the behavior of aqueous solutions under nanoconfinements, the permeability of porous materials, the interactions among graphitic surfaces and their dispersion in aqueous environments. Therefore, our results can be applied to the interface-related phenomena to better understand the interface where the local energy varies at the nanoscales.

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O33. Antimony-lead melts for high temperature electrochemical applications

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Antimony-containing melts are considered as promising materials for high-temperature batteries and energy conversion applications [1]. Potential applications include plastic waste transformation in high temperature reactors to convert the chemical energy contained in organic components directly into electricity [2].

In all these applications, internal resistances must be minimized. In the current work, we, therefore, study the electrochemical oxygen saturation of antimony-lead alloy (50:50 molar ratio) at 700 ^{0}C, to understand electrode mechanisms. Experiments were made in the electrochemical cell shown in Fig.1. A ceramic $Y_{0.8}Ca_{0.2}Cr_{0.95}Ni_{0.05}O_{3\pm\delta}$ disk was used as a current collector, due to offering the properties of high electrical conductivity and chemical stability [3].

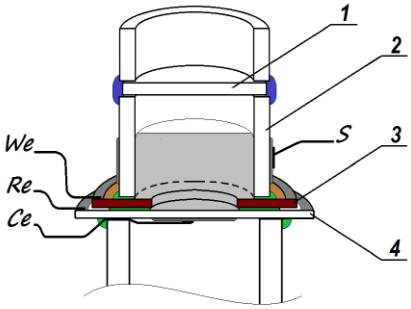

Figure 1. Schematic drawing of the electrochemical cell with melt inside:
1 – Top YSZ disk,
2 – YSZ tube with outer "sensor" electrode (S),
3 – Ceramic current collector in contact with melt,
4 – YSZ bottom pellet with reference (RE) and counter (CE) electrodes

The impedance spectroscopy method was used to assess the resultant polarization resistances of the melt, as it becomes saturated with oxygen. The obtained data are consistent with thermodynamic calculations of the formation of compound forming and segregation in the melt, as a function of melt oxidation [4]. From these results, it is possible to determine the optimal working conditions and limitations for the use of this liquid melt in potential electrochemical applications.

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O34. Photodegradation pathways of Rhodamine B over Gd doped $BiFeO_3$ nanoparticles under solar irradiation

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The purpose of this research is to investigate the photodegradation performance and pathways of rhodamine B (RhB) dye over undoped and Gd-doped $BiFeO_3$ semiconductor photocatalyst using solar irradiation.

Here we have synthesized $BiFeO_3$ and 10 % Gd doped $Bi_{0.9}Gd_{0.1}FeO_3$ (BGFO) nanoparticles following a facile hydrothermal technique at a lower reaction temperature of 160 ℃. Analytical grade $Bi(NO_3)_3.5H_2O$, $Fe(NO_3)_3.9H_2O$ and $Gd(NO_3)_3.6H_2O$ were used as starting materials. The structural, morphological and optical properties of the as-synthesized nanoparticles were characterized by Rietveld refined powder X-ray diffraction patterns, FESEM imaging, Diffuse reflectance spectra (DRS) and Photoluminescence (PL) spectroscopy, respectively. Moreover, the effect of Gd-doping in the properties of $BiFeO_3$ (BFO) such as crystallographic parameters, bandgap, density of states and optical absorption were investigated by first-principles calculations within density functional theory. The photocatalytic performance was investigated by a colorant decomposition test of rhodamine B (RhB) dye under solar light irradiation using a 500 W Xe lamp as a solar simulator.

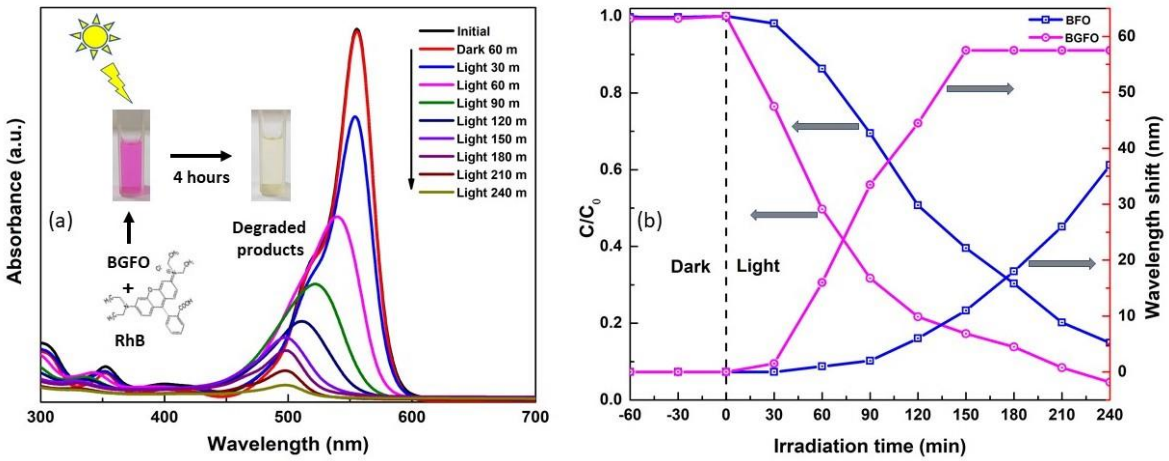

Fig: (a) Spectral changes during the degradation of RhB dye in the presence of BGFO nanoparticles under solar irradiation and (b) A plot of degradation (%) vs irradiation time (min) for BFO and BGFO nanoparticles (black Y axis) and corresponding wavelength shifts in the absorbance band of RhB (red Y axis).

For comparison, a widely investigated photocatalyst, P25 titania nanoparticles have also been subjected to the photodegradation analysis of RhB dye in identical experimental conditions [1]. In order to confirm the stability of the as-synthesized materials, a recyclability test was performed. Also, the active species trapping has been carried out to

determine the most responsible species for the photodegradation of the pollutants over the samples [2].

The BGFO nanoparticles manifest 95% efficiency in degradation of RhB dye, which is higher as compared to the pristine BFO and P25 titania nanoparticles. For both BFO and BGFO nanoparticles a blue-shift in the major absorption band of RhB was observed. In case of BFO the absorbance peak decreases gradually with little blue shift indicating that the cleavage of the whole conjugated chromophore structure was the main pathway. In contrast, for BGFO samples the main absorption band shifts from 553 to 498 nm within 150 min solar irradiation suggesting that N-deethylation was the main pathway for the degradation of RhB [3]. BGFO nanoparticles exhibited good photostability as it did not show sign of deterioration in photodegradation efficiency after four consecutive runs.

Gd doped $BiFeO_3$ nanoparticles synthesized by low temperature hydrothermal method demonstrated high photocatalytic efficiency and excellent stability. The analysis showed that N-deethylation was the key photodegradation pathway of RhB as compared to cycloreversion for BGFO nanoparticles. It is believed that the outcome of this investigation may facilitate better understanding about the degradation mechanisms of RhB and may be beneficial for their potential applications in environmental remediation.

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O35. Synthesis and optoelectronic characterizations of cesium tin chloride ($CsSnCl_3$) perovskite nanocrystals

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Over the last decade, halide perovskites have gained a lot of recognition as a promising class of materials for optoelectronic applications [1]. Especially, the non-toxic $CsSnCl_3$ has intrigued significant interest because of its excellent optical absorption, low charge carrier effective mass and high solar cell potency. To further facilitate the ongoing researches, the structural, optical and photocatalytic performance, as well as theoretical investigations of the optoelectronic properties of lead-free cesium tin chloride ($CsSnCl_3$) perovskite is necessary.

The $CsSnCl_3$ halide perovskite was synthesized by adopting the well-known hot-injection method at low reaction temperature of around 200 ^oC. Herein, the Cs_2CO_3 and $SnCl_2.2H_2O$ were used for the synthesis of $CsSnCl_3$ halide perovskite and oleic acid, oleylamine and 1-octadecene were used as ligands in the chemical reaction. Theoretical results were obtained by using the density functional theory (DFT) based GGA+U function of the CASTEP code.

From the Rietveld refined powder X-ray diffraction (XRD) pattern in Fig. 1(a), we can see that the prepared sample has a crystalline structure with cubic space group *P m-3 m.* No visible surface agglomeration is observed from the FESEM image in Fig. 1(b). The average crystal size was estimated as 300 nm. The thermal stability was investigated using thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC), from which we can confirm that the fabricated sample was thermally stable with a single cubic phase for a broad temperature window up to 280 ^oC. Optical characterization using UV-visible spectroscopy reveals a significantly strong absorbance in the visible spectrum corresponding to a direct bandgap of 2.98 eV, which is well-matched with the reported results [2]. The photocatalytic efficiency of the $CsSnCl_3$ nanocrystals under UV-visible light was recorded as 58% within 180 minutes towards the degradation of rhodamine B (RhB) dye from Fig. 1(c). The structural and optical properties calculated using the GGA+U function of the CASTEP code is in good agreement with the experimental results when U_{eff} = 6 eV. The effective mass of charge carriers in Fig. 1(d) represents the curvature of conduction band minima and valance band maxima for various U_{eff} values. The charge density map confirmed the presence of the Sn-Cl sigma bond in the fabricated nanocrystals.

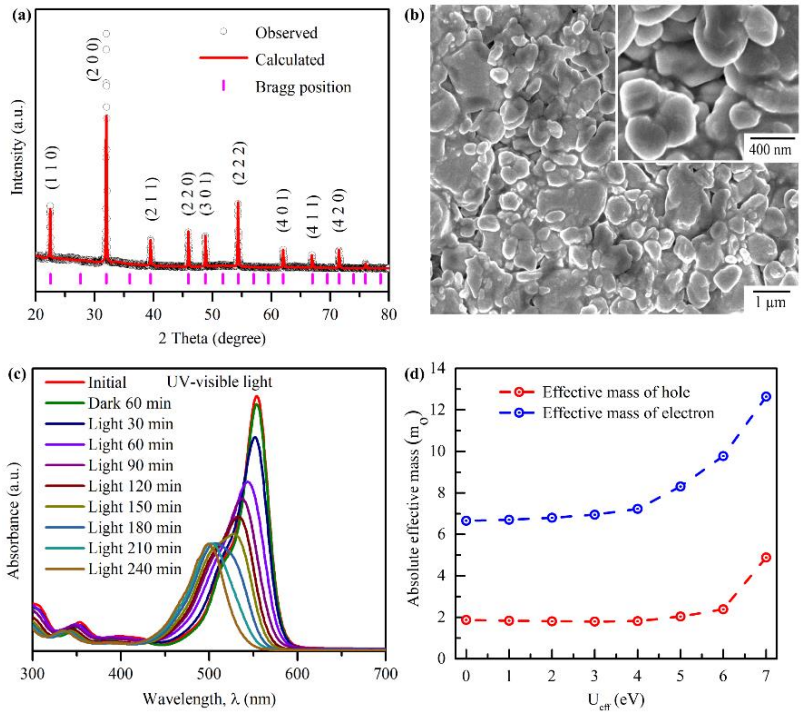

Figure 1. (a) Rietveld refined powder XRD spectrum of $CsSnCl_3$. The XRD spectrum confirms that synthesized $CsSnCl_3$ has cubic lattice formation with the space group of *P m-3 m.* (b) FESEM image of $CsSnCl_3$ nanocrystals. The fabricated sample has no agglomeration. (c) The time-dependent absorption spectra of RhB dye under solar light irradiation. The degradation is 58% within 180 minutes. (d) The effective masses of hole and electron of the $CsSnCl_3$ perovskite as a function of U_{eff}.

The $CsSnCl_3$ perovskite nanocrystals were synthesized using the low-temperature hot-injection method and exhibited good thermal stability without any significant agglomeration. The investigation demonstrated that the photocatalytic efficiency of $CsSnCl_3$ to degrade RhB dye was up to 58 % along the degradation pathway of N-deethylation [3]. The theoretical analysis is in good agreement with the experimental results of the as-prepared sample. The findings of this investigation are expected to contribute to a greater understanding of the cost-effective synthesis process, thermal stability and the photocatalytic activity of lead-free non-toxic $CsSnCl_3$ perovskite nanocrystals.

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O36. Thermoresponsive, pH and redox-sensitive polymer capsules as drug carriers

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The purpose of our experiment is to prepare a poly (N-isopropyl acrylamide) pNIPAM-based capsules composed of a hollow core with high drug loading capacity. The capsule will serve as a drug delivery system, DDS in this case, targeted at cancer cells.
The hollow pNIPAM-based capsules were prepared by precipitation polymerization of NIPAM on sacrificial monodisperse, 3-(trimethoxysilyl) propyl methacrylate (MPS) modified, dimethyldiethoxysilane (DMDES) emulsion templates.[1] To avoid using toxic solvents, ethanol was successfully utilized in the removal of the templates. N, N′-bis(acryloyl)cystine, (BISS) proven to have increased stability, pH sensitivity, and ionic strength[2] over the commercially available N, N′-bis(acryloyl)cystamine, (BAC) was chosen as the polymer crosslinking agent and prepared by us.

The capsules obtained are composed of a core (hollow) and well cross-linked polymer networks with high sensitivity to pH, temperature, and glutathione (GSH) which is a classical and suitable drug delivery system (DDS) for cancer chemotherapeutics.[3] In this experiment, doxorubicin was selected as a model chemotherapeutic, loaded in the capsules, and examined in-vitro at varied pH levels in acetate and phosphate buffer systems with and without GSH.

The results showed a high loading capacity of the DDS and the flexibility of the technique to prepare capsules with additional components, where necessary, and applied for other drugs. The in-vitro drug release studies demonstrated efficient drug release (ca. 90% in less than 4 h) in acetate buffer and 40mM GSH respectively. The pNIPAM-based capsules are biodegradable (supported by the disulfide reduction) and biocompatible with a higher preference over other polymers.

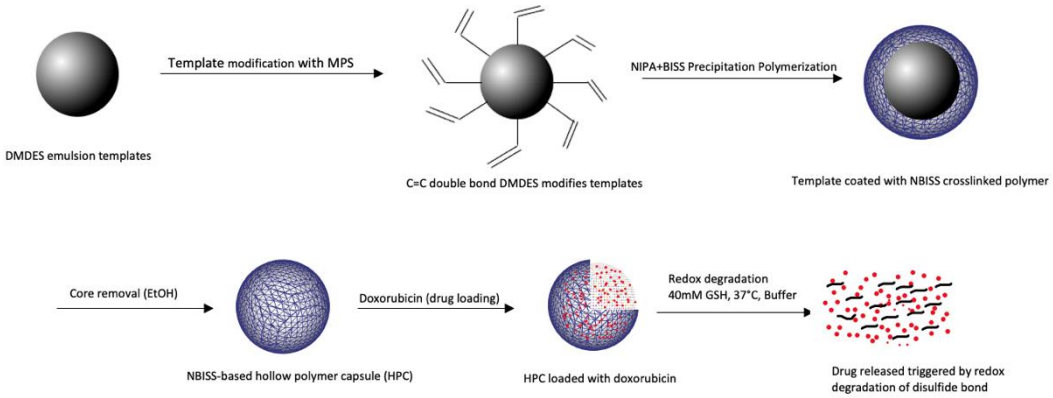

Figure 1: Schematic representation of capsule preparation via sacrificial Silica-based emulsion templates, drug loading, and release via disulfide-bond degradation in typical cancer cell environments.

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O37. RDF-recognition of PtCu bimetallic nanoparticle architecture

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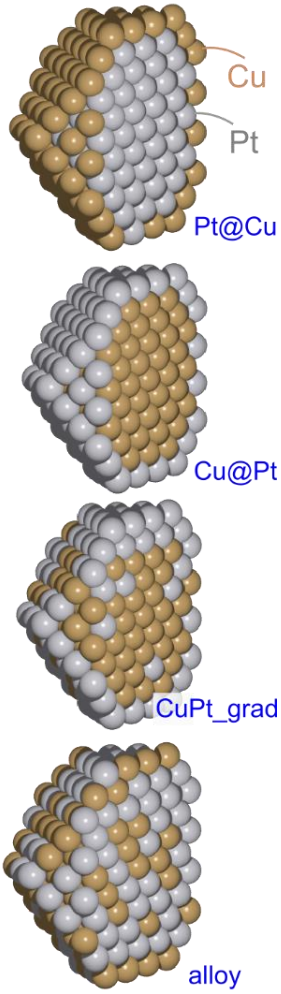
We consider bimetallic Pt-shell Cu-core nanoparticles, which are promising catalyst of oxygen reduction reaction, with activity comparable to that achieved using single-metal Pt particles. Simultaneously, the core-shell particles are more cheap comparing to pure-platinum particles, with higher durability characteristics. Further improvement of durability can be achieved in so called “gradient” nanoparticles with smooth component change in core/shell region.



The identification of the structure (or “architecture”) of bimetallic nanoparticles is not a simple task. It can vary from mixture of independent particles, random solid solution (alloy), core-shell and gradient particles. The difference in the architectures should be reflected in pair radial distribution function of atoms (RDF), which, in turn, can be efficiently measured by X-ray absorption spectroscopy (XAS).

We apply machine learning (ML) algorithms fitted on a synthetic RDF data, obtained from molecular dynamics simulations of nanoparticles with different size, composition and architecture.

We showed high sensitivity of RDF towards the nanoparticles architecture: the correct recognition can be achieved in 99% test cases. The application of ML to RDFs derived for real samples provided expected answers for core-shell and gradient particles, but show high degree of Pt aggregation in PtCu alloy particles. The study is supported by Russian Science Foundation grant # 20-79-10211.

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O38. Hybrid density functional study of iron impurities in hydroxyapatite

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Hydroxyapatite (HAp), $Ca_{10}(PO_4)_6(OH)_2$, is a bio-ceramic material with a calcium-to-phosphorus ratio similar to that of natural bone and teeth. The apatite structure allows the formation of many different compositions, and an easy incorporation of ions in the crystal lattice. The physical, biological, and chemical properties are very sensitive to the details of the electronic structure and changes in it caused by defects and impurities. The understanding of the magnetic properties of Fe-doped HAp [1] requires detailed knowledge of the atomic and electronic structure which can be provided by density functional theory (DFT) simulations.

In the current study we consider single point defects in several charge states, as it was done in the study of the OH vacancy in HAp [2]. The calculations were carried out within density functional theory using Quantum Espresso package to describe the valence states, and ultra-soft pseudopotentials to account for the core electrons. The many-body electronic potential was evaluated using hybrid density functional HSE06 of Heyd, Scuseria and Ernzerhof.

In the calcium-poor conditions Fe_{Ca} substitutions are preferable. If electron chemical potential is high enough then the neutral $Fe_{Ca(II)}$ substitution is expected, otherwise – charged Fe^{+} substitution. Most probable, that Ca(I) charging of the neutral substitution will result in $Fe^{+}_{Ca(II)}$ defect structure.

The study was supported by a grant Russian Science Foundation No. 21-12-00251

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O39. Physical characterization of SiO_2 nanofluid

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Nanoparticles attracted the attention of many researchers a few decades ago. Characterization of nanoparticles properties plays a crucial role in possible application in nanomedicine, diagnostics, cosmetics or printable electronics.

The aim of this work is to characterize LUDOX® colloidal silica nanofluid by using a bit unusual methods, such as density meter and high-resolution ultrasonic spectroscopy (HR-US). Colloidal silica is fine amorphous, nonporous spherical particles suspended in water. The size varies from 7 nm (SM30), 12 nm (HS40) to 22 nm (TM40). The effect of temperature was studied for 25 °C and 37 °C to see if there is any change in density for potential application of the nanoparticles in nanomedicine. Also, water and phosphate saline buffer (PBS) was used for comparison.

DSA 5000 M Density and Sound Velocity Meter was used to study nanofluid density in concentration range from 1 to 30, resp. 40 wt%. High Resolution Ultrasonic Spectroscopy is a non-destructive real-time method to study intrinsic properties of liquid using ultrasound waves. It gives information about conformational transitions of polymers, ligand binding, self-assembly and aggregation, crystallization and gelation, monitoring of bio-chemical etc. [1]. Combining these two methods allow us to calculate nanofluid compressibility, an important property for further application.

We found out that density increases linearly with nanofluid concentration. The effect of temperature and solvent was not negligible. Calculated compressibility decreases linearly with concentration. This is very interesting because measured ultrasound attenuation, used for compressibility calculation, decreases first up to 15 wt% and increases afterwards.

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O40. The influence of ammonolysis temperature and time on synthesis of cubic niobium (oxy)nitride

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Interest in ammonia (NH_3) is increasing due to its application in a large number of products and its potential to be used as an alternative carbon-free fuel that can play a crucial role in a sustainable energy future. The current industrial process for NH_3 synthesis is the Haber-Bosch process (HBP). However, this process is estimated to be responsible for 2.5 % of worldwide greenhouse-gas CO_2 emissions, due to its reliance on hydrogen sourced from natural gas[1–3]. To solve this problem, research has been focusing on the development of alternative, sustainable, technologies, where one of the most promising is the direct electrochemical synthesis of NH_3 from steam and nitrogen[4]. A critical challenge to the success of this process is to find a suitable electrocatalyst for nitrogen reduction reaction (NRR), due to the competition of NRR and hydrogen evolution reaction (HER) that take place at the cathode[1,5]. Transition metal nitrides, namely, niobium nitride (NbN) has been highlighted by DFT calculations to potentially offer high catalytic activity for the ammonia formation reaction, whilst suppressing H2 evolution (HER)[6,7].

A pure phase of the cubic NbN composition can be obtained from niobium pentoxide (Nb_2O_5) by a thermal ammonolysis route[8]. In this work, we, therefore, study the influence of temperature and time on the crystal structure, microstructure, and nitrogen content of cubic system of niobium oxynitride, using different techniques such as X-ray diffraction, X-ray photoelectron spectroscopy, Scanning Electron Microscopy and thermogravimetry.

Acknowledgements

The authors acknowledge to FCT for the PhD grant SFRH/BD/130218/2017 and the projects, PTDC/CTM-CTM/2156/2020, PTDC/QUI-ELT/3681/2020, POCI-01-0247-FEDER-039926, POCI-01-0145-FEDER-032241, UIDB/00481/2020 and UIDP/00481/2020 and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF).

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O41. $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ as electrocatalyst for the electrochemical promotion of N_2O reduction

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Nitrous oxide (N_2O) is a green-house gas responsible for several environmental problems, such as photochemical smog, acid rain, ozone layer depletion and global warming [1].

By bridging the solid-state chemistry with heterogenous catalysis, the aim of the current work is to study the non-Faradaic electrochemical modification of catalytic activity (NEMCA) [2] of the N_2O reduction reaction, using $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ as electrocatalyst. This double perovskite is a very promising mixed ionic-electronic conductor (MIEC) reaching 0.13 S cm^{-1} of oxygen ionic conductivity at 800 °C as well as high structural stability in both reducing and oxidizing conditions [3]. In this work, SFMO material was successfully synthesized by sol-gel method as confirmed by X-ray diffraction (XRD).

A single pellet reactor was developed, made of 8YSZ electrolyte, SFMO as working electrode and gold (Au) as counter and reference electrodes. Aiming to prevent the inter-reaction of YSZ with SFMO, a $Ce_{0.9}Gd_{0.1}O_{2-\delta}$ (CGO) was used. From the experiments, it was found that by applying cathodic polarisation (*i.e* -0.05 and -0.25 A), an increase of the catalytic rate (r O_2 mol s^{-1}) was observed, resulting in a significant increase of N_2O conversion (Figure 1). The enhancement factor, also known as Faradaic efficiency (**Λ**), was also calculated for the tested experimental conditions, showing values > 1, demonstrating the non-Faradaic electrochemical behaviour. Particularly, at 700 ºC, a **Λ** value of 4.2 was obtained at the lower current tested (-0.05 A). Additionally, the nature of the mechanism was also assessed, showing a completely reversible effect, where the electrochemically promoted reaction rate returns to its open circuit (unpromoted) value upon removal of polarisation (Figure 1).

This work, therefore, evidences that non-Faradaic activation of heterogenous catalysis can be an effective and very useful tool to promote the reduction of this greenhouse gas, with high environmental importance.

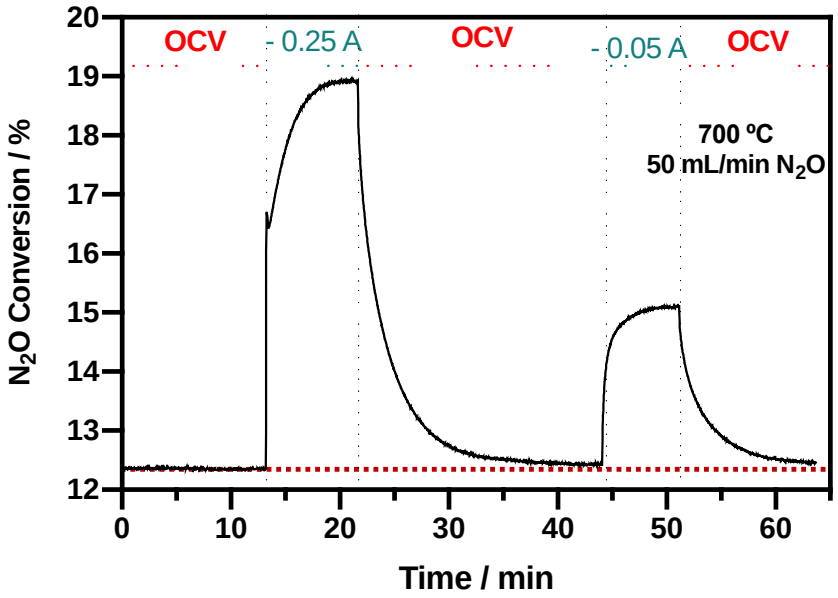

Figure 1 – N_2O conversion as function of time under polarization (-0.25 and -0.05 A) and OCV conditions.

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O42. Temperature-dependent mixing behaviors of Bi -Mg liquid alloys

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Bi - Mg is a strongly interacting system (the free energy of mixing G_M > 3 RT at equiatomic composition), the compositional dependence of the thermodynamic properties (free energy of mixing, heat of mixing and entropy of mixing) exhibit asymmetric behavior about equiatomic composition and are in well agreement with experimental data literature. Such an interesting feature is explained here through complex formation model on the basis that a complex of the form Bi_2Mg_3 exists in the bulk phase. Its energetics is used to investigate the structural properties (concentration fluctuation in long wave length limit and chemical short range order parameter) and the transport property (ratio of mutual diffusion coefficient to intrinsic diffusion coefficient). The mixing behavior of Bi – Mg system is further explored through the study of coefficient of viscosity, surface composition and surface tension. Our study indicates that the surface is enormously rich with Bismuth concentrations throughout the composition of the alloys.

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O43. Magnesium hydride-added titania anode for Li-ion battery

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

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O44. Quantitative measurements of the piezoelectric coefficients using “global-excitation” mode of the piezoresponse force microscopy

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Piezoresponse force microscopy (PFM) is a local technique allowing measurement of the surface piezoresponse with a uniquely high spatial resolution in the micro and nano-objects where macroscopic measurement techniques fail and PFM becomes the only way to quantify the material's piezoelectric coefficients. In the case of using the typical PFM mode with an application of the electric field to the scanning probe microscopy probe, the measurements are realized in the conditions of the highly non-uniform electric field. This leads to many uncertainties in the measurements, such as a significant impact from the electrostatic force, the drop of the applied voltage across the tip-surface interface, mechanical clamping of the oscillating surface, etc. Another straightforward PFM implementation is in the so-called "global-excitation" mode, where an electric field is applied through micro- or nano-sized electrodes, while signal registration is performed utilizing scanning probe microscopy probe rastering across the surface. Global excitation can be realized via an electric field applied to the conductive tip across the tip-electrode interface and simply by the excitation of the electrode and probe acting as a mechanical sensor. In both cases, the solution of the problem of electromechanical response quantification in the applied electric field is close to the conventional laser interferometry problem of the response under the action of the uniform or close-to-the uniform electric field. In this talk, we discuss the experimental implementation of the "global-excitation" mode PFM for the quantitative probing of the piezoelectric coefficients at the micro- and nanoscale. As well as we introduce the accurate analytical solution for the "global-excitation" mode PFM task. Current studies are essential for the development of novel piezoelectric materials useful in various applications.

The equipment of the Ural Center for Shared Use “Modern Nanotechnology” UrFU was used. The work is supported by the Russian Science Foundation (grant 19-72-10076).

O45. Nanodiamonds as a treatment for organophosphate poisoning

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Nanoscience drastically changed our classical understanding of chemistry, biology, physics, and molecular interactions, allows us to try new pathways for drug delivery and use of bioactive compounds for nanomedicine.

In recent years, different carbon nanoparticles (CNP) were used for biomedical applications [1]. They were studied as a potential treatment, as well as a drug delivery platform. In this study, we used the nanodiamonds (NDs) which showed the least toxicity amongst other CNP [2]. The powder made of ca. 5nm diamond particles with large accessible surface and tailorable surface chemistry shows extraordinary optical, mechanical, electronic, and thermal properties on the nanoscale. Inert and biocompatible NDs could be used in nanomedicine and biotechnology to improve the therapeutic value of various drugs [3].

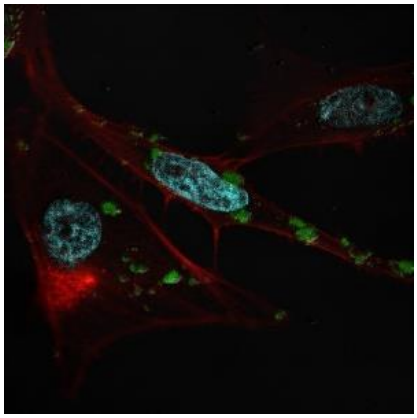

Fig.1. Localization of Nanodiamonds in the cell.

We tried to design the most beneficial method of the preparation of drug-coated harmless NDs for treatment of organophosphate poisoning. Developing potent antidotes towards acetylcholinesterase (ACHE) inhibited by OP in the central nervous system remains a challenging task. Continuing our previous work on design of oxime-functionalized reactivators [4], we synthesized several bioactive compounds and purified them, followed by attaching/coating on NDs' surface. The modified NDs were studied by different techniques (ssNMR, FTIR, DLS, SEM) and tested in the collaborator's biomedical laboratories for reactivity towards inhibited ACHE and toxicity screening against the mammalian cells. Its permeability across the blood-brain barrier was carefully investigated.

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O46. Intercalation of C_{60} fullerite films by yttrium atoms

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Alternative non-hydrocarbon energy is actively developing today. Hydrogen energy is one of the directions of alternative energy. Finding efficient storage media for hydrogen is a challenging task for researchers to provide an advancement of hydrogen and fuel-cell technologies. Carbon-based nanomaterials, in particular, fullerenes are considered to be the promising candidates for hydrogen storage. Though the hydrogen storage capacity of pristine fullerenes is low, but it can be sufficiently enhanced by decorating them with suitable metal atoms. However, the big problem for these decorating systems is associated with the metal clustering. Unfortunately, metal clustering either above or beneath C_{60} layers was found to be typical for many metals. The recent theoretical work [1] predicted that decorating C_{60} molecules with Y atoms can cause a remarkable enhancement in the hydrogen adsorption capacity. It is worth noting, however, that any experimental data on Y interaction with fullerenes are lacking. In particular, it remains unknown if Y atoms agglomerate into clusters or not upon adsorption at the C_{60} layers.

We report on the results of the scanning tunneling microscopy observations of Y adsorption onto the C_{60} fullerite films grown on the Au/Si(111)-α-$\sqrt{3}\times\sqrt{3}$ surface. It was found that Y atoms avoid clustering and become incorporated into the fullerite film as individual atoms. Tight binding of Y atoms in their sites provides a principal possibility for growing the fullerite films with arbitrary in-depth Y doping profiles using appropriate successive depositions of Y atoms and C_{60} molecules. Yttrium atoms transfer the charge to the three neighboring surface fullerenes making them looking bright in the filled-state STM images. A promise that the heavily Y-doped C_{60} layers might possess properties of the hydrogen storage medium. To test this possibility, further experimental researches are required [2].

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O47. Fabrication and simulation of electrodynamic properties of ZnO nanowires coated with Ag beads for sensing applications

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Design/engineering of a versatile platform for detection of trace amounts of polluting contaminants, biomarkers of diseases or drug molecules by surface enhanced Raman scattering (SERS) spectroscopy is an ultimate goal of state-of-the-art sensing technology. Current SERS-active platforms provide attomolar detection limit [1] giving a rise to focus on the new key point indicators of high reliability of the SERS assay and its affordability for the end-user. In these terms, ordered arrays of plasmonic nanoparticles (NPs) on photocatalytically active metal oxides, which can potentially be self-cleaned for reuse, attract particular interest. In this work, we fabricated and characterized ZnO nanowires (NWs) coated with Ag beads (Fig. 1, a) possessing prominent SERS-activity and nanomolar detection limit for small organic molecule (R6G). Oxidized Si wafer was used as an initial substrate for magnetron sputtering of 100 nm ZnO seed layer and further thermal evaporation of Ag NPs (~35 nm in diameter). Then ZnO was hydrothermally deposited on the Ag-coated seed layer from $Zn(NO_3)_2 \cdot 6H_2O$ and NaOH solution at 80°C for 30 min. ZnO NWs coalesced into bundles after hydrothermal synthesis were coated with Ag beads by thermal evaporation. The 3D geometry of the experimental sample was studied with COMSOL Multiphysics 5.3 to simulate electric field strength distribution (Fig. 1, b). The major contribution into the Raman signal enhancement was found to be provided by the Ag NPs at the bottom of the ZnO NWs but Ag beads were a source for inter reflection between them. The latter opens prospects for the reliable detection of macromolecules, which can be completely overlapped by the reflected light.

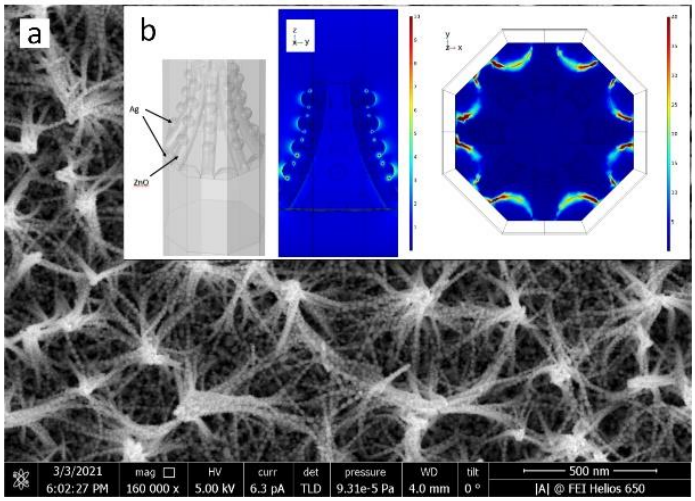

Fig.1 SERS-active substrate based on ZnO NWs coated with Ag beads: (a) SEM top view and (b) simulations of 3D geometry and electric field strength distribution.

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O48. Increasing the photoactivity of titanium oxide nanotubes by heat treatment in glycerin

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The growing pollution of the environment due to the use of traditional energy sources is forcing humanity to look for new ways to obtain environmentally friendly energy. One of such energy sources can be hydrogen - a clean, cheap and widespread element in nature. One of the most promising sources of its production is the photocatalytic decomposition of water under sunlight into H_2 and O_2. TiO_2 nanotubes (TNT) arrays are a promising tool for use as a photocatalyst. However, they have disadvantages such as poor charge carriers separation and limited UV absorption.

An increase in the photocatalytic activity of TNT is possible due to an increase in the efficiency of separation of photogenerated charge carriers. This can be achieved by creating p-n junctions in the structure and on the surface of the tubes, which, due to the internal field, will facilitate the separation of electrons and holes. One of the materials for creating a p-n junction can be copper oxide, which is introduced into the tube structure in various ways [1].

In this work, TNTs obtained in a solution of a fluoride-containing electrolyte were modified with copper acetate using glycerol heated to 200°C as a solvent.

Measurement of the optical band gap by the Kubelka-Munk method showed a decrease in the optical band gap. The results of measuring the photocurrent show that after modification of the structure, an increase in photoactivity is observed in both the visible and UV regions.

The results of this work can be used for further research in the field of increasing the photocatalytic efficiency of materials based on TNT.

Acknowledgments: the study was carried out with the financial support of the Russian Foundation for Basic Research within the framework of the scientific project No18-29-23038 MK and the state assignment for 2020-2022 of the Agreement FSMR-2020-0018.

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O49. Development of a dispersion preparation process based on Al-Ni-FeOx nanopowders for direct ink writing of energetic materials

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One of the options for increasing the efficiency of the thermoelectric device [1] is the optimal distribution of the energetic material over the surface of the thermoelectric generator (TEG). One of the ways to solve this problem is to apply a composite energetic material by printing using a stable dispersion with the required viscosity. However, to implement this technique, it is necessary to solve a number of technological problems associated with the elimination of cracking of the material after drying, the creation of reliable adhesion between the composite and the substrate.

For improving adhesion, to exclude cracking of the energetic material layer after application, a dispersion was used, consisting of isopropyl alcohol and Al / Ni / FeOx nanopowders, with the addition of carbon nanotubes (CNTs) and Pattex Classic glue. Carbon nanotubes act as a dispersion stabilizer, being distributed throughout the solution volume, they create a retaining framework for nanoparticles. When the dispersion dries, the adhesive ensures reliable adhesion of the material to the TEG surface. The formed layer of energetic material after drying contains no more than 5 wt.% of functional additives, which bind 95 wt.% Of nanothermite.

The precision application of dispersions was carried out using a Nordson robot dispenser, which allows you to control the amount of applied material per unit surface. This method provides the application of an energetic material with the required topological pattern and a certain mass on the TEG surface at a high speed without human intervention.

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Poster presentations

P1. Corrosion resistance of Cor-Ten steel in different environments

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Construction materials exposed to atmospheric conditions are often subject to corrosion and need to be protected or prevented from further corrosion [1]. The aim of this paper was to determine the behavior of the weathering steel Cor-Ten in different media: distilled water, acid rain and seawater during the three months. Cor-Ten steel got its name because of its corrosion resistance and tensile strength properties. It is available as Cor-Ten A and Cor-Ten B [2]. Corrosion morphologies were observed by stereomicroscope while the changes of samples and shape of corrosion products and their adhesion to the material were monitored by the visual method. Also, mass loss of samples was measured and corrosion resistance of the Cor-Ten was estimated by electrochemical impedance spectroscopy (EIS).

These results show that the microstructure of Cor-Ten steel is fine-grained and slightly directed; it is composed of ferrite and perlite. The surface of exposed samples to distilled water was the least corroded, while the effect of corrosion was most pronounced in samples exposed to seawater. All tested samples had obvious nonuniform corrosion and the formation of solids products in the form of flakes. There was no change in the mass of the samples in distilled water and acid rain, while in the samples in seawater there was a very small loss of mass. The obtained EIS results showed that the surface of Cor-ten steel starts to be reactive with exposure to aquatic mediums, which is different from the scientific literature for this material [3]. Cor-ten steel passivates itself by creating an oxide layer on its surface, and for this reason, no additional protection of its surface is required.

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P2. Effects of microstructural orientation on bending strength in the longitudinal direction of pedunculate oak

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Wood is a natural building material that is heterogeneous and anisotropic structure and therefore has different properties. The properties may vary depending on the species, but also the anatomical structure of the trees within the species, where they may have ten times lower density in some parts or several times higher bending strength, hardness or stiffness. Bending strength is the resistance of a material to the action of an external force that seeks to bend and break it. For wood, this mechanical property is extremely important, and the value of bending strength depends on the orientation of the wood structure, where the highest value is in the longitudinal direction. For some types of wood, the bending strength also depends on the angle closed by the bending force and annual rings [1, 2].

This study shows the results of testing the bending strength of pedunculate oak (*Quercus robur* L.) in the longitudinal direction using a three-point bending method. The angle between the bending force and the lines of the annual rings was 0°, 45°, and 90° (Fig. 1). It has been shown that the position of the bending force in relation to the direction of the annual rings slightly affects the value of the bending strength in the longitudinal direction. The highest value of bending strength is obtained for angle 0° (175.30 N/mm^2). The values for angles 45° (172.61 N/mm^2) and 90° (173.24 N/mm^2) are very similar. The dissipation of the results is described with the Weibull distribution, which is confirmed to be suitable for the statistical analysis of the results obtained [3]. For a group of samples with a 45° angle, the value of the Weibull modulus is the highest, indicating the highest homogeneity of the structure.

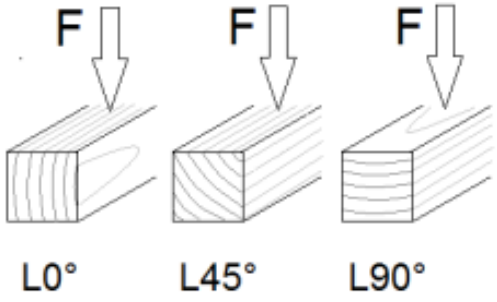

Figure 1. The direction of load in relation to annual growth ring orientation [4].

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P3. The mechanical behaviour of concrete with chicken feather fibres at high temperature

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The aim of this work is to improve the mechanical behaviour, especially when pulling high temperature fibre concrete. In our study, we used polypropylene fibres (FPP) in quantities of 0.15% of the volume of concrete and chicken feather fibres (FCF) in quantity of 0.05% of the volume of concrete. The test pieces shall be heated to temperatures between 150°C and 750°C with a temperature increase of 1°c/min, the results indicate that the residual tensile strength of the concretes reinforced by fibres from poultry feathers is higher than that of the concretes reinforced by fibres polypropylenes.

P4. Effect of long baffles on forced convection heat transfer over multiple heated blocks

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The forced convection heat transfer over five heated blocks in a horizontal channel contains long baffles fixed at the upper wall, is investigated. The finite volume with Ansys Fluent © code is used as a numerical analysis tool. Simulations are performed for two cases with and without baffles. The study is limited to a steady-state and the calculations are run in an unsteady scheme to avoid unrealistic results and ensure that the flow still steady under the simulation conditions. The dimensions of the blocks are considered the same (w=h=0.5), the cooling process is done with air (Pr=0.71). The streamlines, isotherms, and the local Nusselt are illustrated to show the effect of the long baffles on the fluid flow, temperature, and heat transfer in both fluid and solid phases. The results show that the long baffles cause a significant heat transfer enhancement over the blocks due to changes in the flow behaviors.

P5. Cobalt oxyhydroxide nanoflakes-reduced graphene oxide nanocomposite based Electrochemical detection platform for determination of flunitrazepam in biological samples

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Monitoring of benzodiazepine, a class of psychoactive drugs in biological matrix is still a challenging task due to low concentration and ease of biotransformation. Therefore, there is an utmost requirement of exploration of suitable electrode nanomaterial having excellent conductivity, high specific surface area, good catalytic ability, and chemical stability for potential application in electrochemical sensor. Introduction of novel 2D nanomaterial such as cobalt oxyhydroxide nanoflakes on the rGO surface may result into fabrication of highly conductive electrochemical sensor for flunitrazepam detection. The applicability of screen printed electrode modified with CoOOH nanoflakes and reduced graphene oxide nanocomposite offers promising results due to synergistic effect between CoOOH and rGO compared with conventional nanocomposite comprising zero dimensional nanoparticles and 2D rGO. Therefore, the present work focuses on the development of flunitrazepam sensing platform based on cobalt oxyhydroxide nanoflakes-reduced graphene oxide nanocomposite (CoOOH-rGO). Validation and testing of the developed sensor for relevant drug samples in biological matrix demonstrated the robustness of such platforms. Further, excellent electrochemical performance of the sensor confirmed the plausibility of using the above technique in point-of-need screening of flunitrazepam and suggest that CoOOH-rGO nanocomposite holds promise as an effective analytical tool to prevent phenomena of covert drug administration.

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P6. Use of infrared temperature sensor to estimate the evolution of transformation temperature of SMA actuator wires

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1. Introduction

Shape memory alloys (SMAs) can be used as actuators with application of temperature gradients, altering material's crystallographic phase while it reaches transformation temperatures, and it extends macroscopically [1]. It's possible to measure temperature of SMA with any standard temperature measuring instrument, except when used on small size scales, such as actuator wires. In this work, we attempted to focus an infrared (IR) sensor on a thin SMA wire with 0,150mm diameter and measure its temperature during thermal cycling procedures, characterizing some material thermal properties.

2. Results

The main result is shown in figure 1.

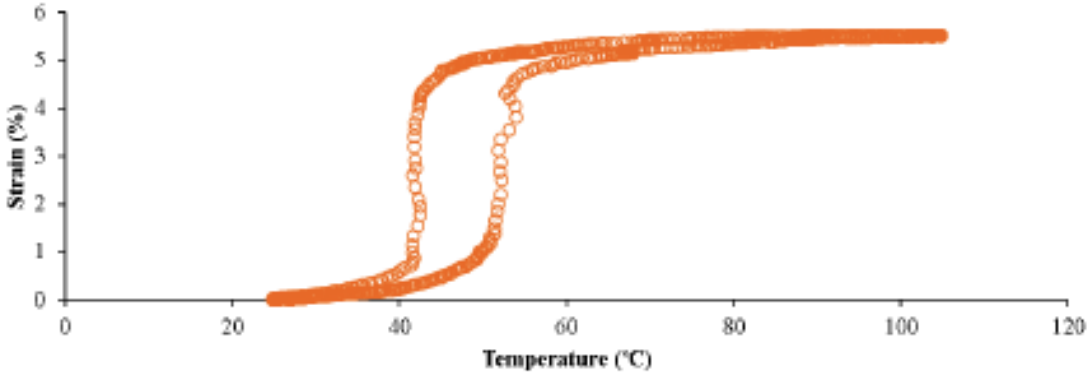

Fig. 1: Early hysteresis loop of a NiTi alloy subjected to thermal cycles and 150 MPa stress. Temperature is measured with IR temperature sensor.

Tangent lines in the hysteresis loops give the value of the phase transformation temperatures of the specimens: M_f =41.4ºC, M_s =44ºC, A_s =49.7ºC and A_f = 55.8ºC.

3. Conclusions

IR sensors can be used to estimate temperature of thin SMA actuators, despite its difficulty to focus. Any movement disorder between the sensor and the specimen resulted in oscillation in hysteresis loops plots. Differential scanning calorimeter (DSC) can be used to estimate the transformations temperatures of the material when no stress is applied, then its results can be used to compare this work results.

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P7. Measuring systems for investigating the physical properties of superconducting materials

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When investigated high-temperature superconductors, special attention is given to the devices and research methods to investigate the physical processes ongoing in superconductors. To realize the well-known HTS investigated methods: magneto-mechanical, optical, Mossbauer, radio technical, Etc., a proper stable low-temperature environment making device – cryostat is required. It represents a hermetic chamber isolated from the environment, where a low temperature can be achieved and maintained for a long time.

This paper presents a cryostat created in our laboratory with a working temperature range of 65-300K, which is associated with investigating the physical parameters of high-temperature superconducting materials.

To achieve these goals was created a basic cryostat with four replaceable modules for studying: physical properties of superconductors; superconductors in high critical currents; superconductors in strong magnetic fields; Low field electrodynamics in superconductor materials. For investigated the physical parameters of materials mainly used three methods: a four-probe method for measurements of electrical resistivity and value of the high critical current density; linear ac susceptibility $\chi=\chi'+i\chi''$ and nonlinear susceptibility χ_n. This cryostat makes it possible to measure this parameter at different values of temperature, ac and dc magnetic fields, and the frequency of the alternating field.

Acknowledgments
This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG), under GENIE project, grant number: CARYS-19-1832, Project title: Innovative Cryostat for Studying High-temperature Superconductors.

P8. A first-principles study on the electronic and optical properties of Nd_2FeCrO_6 double perovskite

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The purpose of this research is to investigate the electronic and optical properties of Nd_2FeCrO_6 (NFCO) double perovskite theoretically using the Cambridge Serial Total Energy Package (CASTEP) [1].

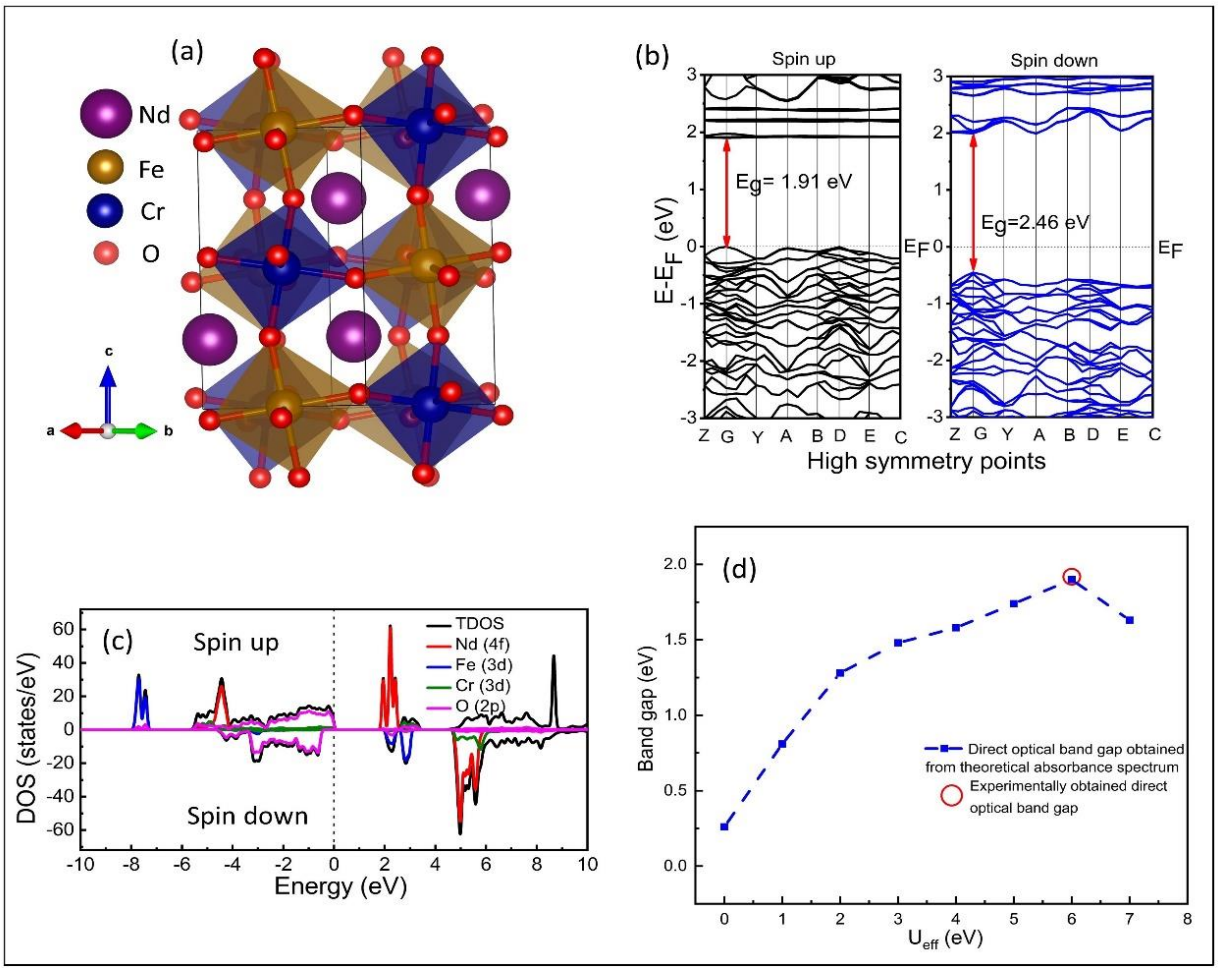

Fig. (a) Schematic representation of the Nd_2FeCrO_6 monoclinic unit cell with its (b) band structure and (c) total density of states and partial density of states of Nd-4f, Fe-3d, Cr-3d and O-2p orbitals for U_{eff} = 6 eV. (d) Variation in theoretically calculated direct optical band gap as a function of U_{eff}. The red circle in fig (d) represents the experimentally obtained optical band gap value.

Recently, we have synthesized NFCO nanoparticles for the first time by a facile low-cost sol-gel citrate method. Several double perovskites have been reported to possess promising applicability in the field of photocatalysis, photovoltaic devices and photo(electro)chemical energy storage systems [2,3,4]. Here, we have used both generalized gradient approximation (GGA) and GGA+U methods within the plane-wave

pseudopotential framework by employing experimentally obtained structural parameters. To the best of our knowledge, no experimental or theoretical characterizations of NFCO double perovskite have been reported yet.

In this investigation, we have reported the spin-polarized electronic band structure, charge carrier effective masses, density of states and electronic charge density distribution as well as the optical properties of NFCO double perovskite. Furthermore, the impact of on-site Coulomb interaction energy (U_{eff}) on electronic and optical properties was also explored using GGA and GGA+U methods to apply a number of Hubbard U_{eff} parameters to the Fe-3d and Cr-3d orbitals varying from 0 to 7 eV. Mulliken population study confirms the existence of ionic and covalent bonds in NFCO perovskite, revealing that the Cr–O and Fe–O bonds are more covalent than the Nd–O bond. Notably, the band structural analysis reveals that NFCO double perovskite is a direct band gap semiconductor. For U_{eff} = 6 eV, the measured electronic band gap for majority spin states is 1.91 eV. It was observed that theoretically calculated direct optical band gap was 1.90 eV for U_{eff} = 6 eV, which is marginally less than the experimentally obtained optical band gap of 1.95 eV. As a result, we propose applying a U_{eff} value of 6 eV to the Fe-3d and Cr-3d orbitals in NFCO to investigate accurately its optical and electronic properties.

The outcomes of our investigation highlight the importance of conducting systematic investigations into the effects of the U parameter not only on band gaps but on the electronic structure as a whole, especially for highly correlated materials.

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P9. Free vibration analysis of functionally graded SWNT

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In the present study, an analytical method is used to investigate the free vibration of functionally graded single-walled carbon nanotube. The Timoshenko beam model is used. In order to model the nanostructure Eringen's nonlocal elasticity is employed. The governing equations and boundary conditions are derived according to Hamilton's principle and the obtained results are determined by the analytical method.

After the validation of our results with previous studies, numerical results are presented to figure out the effects of nonlocal parameter, rotating inertia, and the material effect on the natural frequencies of the nanotube.

P10. Experimental and theoretical study of carbon micro- and nano-spheres doped by nitrogen

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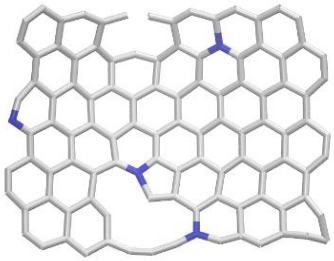
Carbon materials are interesting objects both from fundamental and applied points of view [1]. Magnetic carbon materials (with magnetism due to the s- and p(π)-electrons) are promising for biomedical applications (bio-compatibility, low mass density and good plasticity).



We consider room temperature ferromagnetic carbon materials obtained as a result of solid-phase pyrolysis [2] of metal-free phthalocyanine. Pyrolysis products of metal-free phthalocyanine contained 1 - 4 at. % N, which replaces carbon in the graphene lattice, probably, in pyrrolic and pyridinic coordinations. The sample with 4 at. % N demonstrates a strong paramagnetism in the temperature range of 5-300 K, with a temperature dependence similar to ferromagnetic cluster spin-glass. To reveal the origin of these ferromagnetic properties, atomic structure of the synthesized carbon spheres is studied and determined using transmission electron microscopy, X-ray diffraction, X-ray photoelectron and X-ray absorption spectroscopy in combination with molecular dynamics simulations. The relationships between the pyrolysis conditions (temperature, pressure, duration of pyrolysis, reagent for pyrolysis) – atomic structure of the N-species, their type and concentrations in the mean carbon's sphere – and the observed magnetic characteristics of the sample are established. This will allow to improve the magnetic characteristics of carbon spheres by governing and optimizing the concentration of impurity nitrogen atoms and carbon edge states with zigzag type in graphene clusters by changing parameters of pyrolysis. The study is supported by RFBR grant # 20-52-05011.

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P11. Vibration study of a piezoelectric nano-shaft

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The aim of this work is to find the natural frequencies of a rotating piezoelectric nano-shaft before finding the critical system speeds using a Campbell diagram.

We used the beam theory of Euler Bernoulli [1] to describe the stress and strain displacement fields. From the theory the non-local elasticity [2] constitutive relation of the piezoelectricity [1] one resulted in extracting the strain and kinetic energy and the work of external forces [3] we find our differential equation from Hamilton principle**.** To solve our equation to find the natural frequencies we used the analytical state space method [4].

For test the efficiency of our method used state space we tried to find the natural frequency. The studied structure is of steel beam type with the following dimensions and characteristics: Length L=250mm, width b=20 mm and thickness h=0.5 mm [5]. Young's modulus E=21.1010 N/mm², Poisson coefficient 0.3, Volumic mass 7800 kg/m3 am of Euler Bernoulli in simple bending. We compared with Deghboudj Samir [5] which is calculated with an analytic method and a simulation using ABAQUS.

These results of vibratory analysis of a piezoelectric rotary nano-shaft can be used for the design of nano-scale rotary devices.

Table 1: Comparison of 3 first natural frequency of a beam of Euler Bernoulli.

	Vibration mode	First	Second	Third
[5] analytic	Frequency (Hz)	6.704	42.037	117.519
[5] abaqus	Frequency (Hz)	6.9871	43.7290	122.4600
present	Frequency (Hz)	6.5276	41.7636	113.8619

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P12. Crystal structure and magnetic phase transitions in $BiFeO_3$ -based ceramics driven by high pressure

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Over the last decades, ferrites and manganites have attracted great attention of scientific society. Especially the compounds with chemical composition near the phase boundary as they are characterized by metastable structural state. Metastable structural state provides a frustration of ferroic orders which opens up new possibilities for practical applications of the $BiFeO_3$-based multiferroic materials.

Samples of the $Bi_{1-x}Sm_xFeO_3$ system with dopant ion concentrations up to x = 0.20 were prepared by the sol-gel reaction method. Structural measurements for the compounds $Bi_{1-x}Sm_xFeO_3$ have confirmed the presence of structural transition from the rhombohedral phase to the nonpolar orthorhombic phase through the formation of the antipolar orthorhombic phase. The mentioned series of the phase transitions occurs upon increase in the dopant content, heavily doped compounds are characterized by a stabilization of the nonpolar orthorhombic phase. An application of external pressure (P ~ 5GPa) to the compounds having chemical composition within the phase boundary region leads to significant modification of the crystal structure and magnetic properties. Thus, an application external pressure leads to a stabilization of the orthorhombic states, viz. the polar rhombohedral phase diminishes and transforms to the anti-polar orthorhombic phase (Fig. 1), while the anti-polar orthorhombic phase transforms to the non-polar orthorhombic phase. Magnetic properties of the compounds subjected to external pressure demonstrate an increase in the magnetization of the compounds having dominant rhombohedral phase, wherein coercivity significantly increases, while the spontaneous magnetization remains nearly constant.

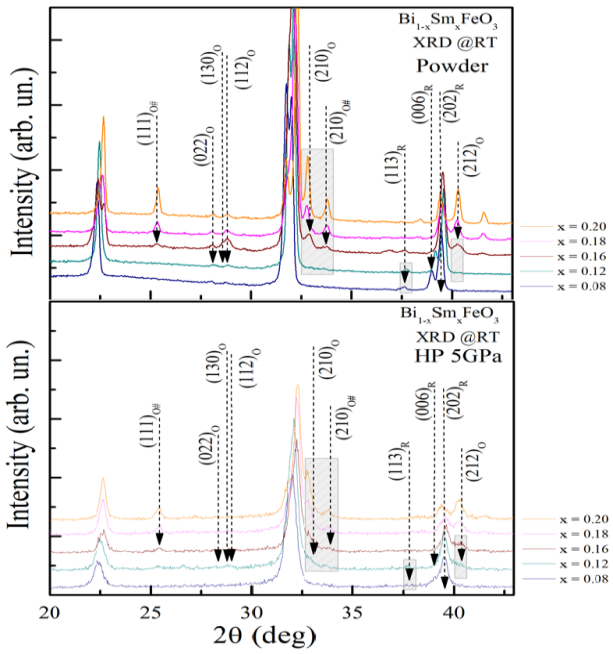

Fig.1. X-ray diffraction patterns of $Bi_{1-x}Sm_xFeO_3$ (x = 0.08, 0.12, 0.16, 0.18, 0.20) for powders (upper) and tablets obtained after high pressure (5 GPa).

The research was supported by BRFFR and RFBR (projects # F20R-123, # 20-58-00030).

P13. Plasmonic nanostructures based on the metalized porous silicon for SERS

K. Girel[1,4*], A. Burko[1,4], S. Zavatski[1,2,4], N. Khinevich[1,3], S. Dubkov[4], A. Savitsky[4], D. Novikov[4], A. Tarasov[4], H. Bandarenka[1,4]

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Surface-enhanced Raman spectroscopy (SERS) is a special technique of Raman spectroscopy, which allows significantly increased of the Raman signal from molecules adsorbed on the noble metals nanostructures surfaces [1]. Enhancement of the Raman signal from analyte molecules occurs due to the localization of surface plasmons in metal nanostructures and an increase of their electromagnetic field under the influence of the exciting radiation [2]. In this work, we propose a method for the SERS-active substrate formation based on Ag nanoparicles on the surface of macroporous silicon (macroPS) coated with a continuous Ni film. MacroPS with a pore depth of 1–2 μm and a diameter of 1-1.5 μm was formed by the electrochemical anodizing of the surface of p-type monocrystalline silicon in a solution containing hydrofluoric acid (HF). A 0.8 μm thick nickel film was formed by electrochemical deposition. The formation of silver nanoparticles was carried out by the method of chemical deposition from silver nitrate aqueous solution with HF. It was revealed that the Ni film surface is covered with a layer of ellipsoidal Ag nanoparticles with a high degree of polydispersity (Fig 1(A)). A gradient of average Ag nanoparticle sizes from the center to grain boundary of the nickel film is observed. It is shown (Fig.1(B)) that structure has a large band of surface plasmon resonance due to polydispersity of the silver particles. Due to wide band of plasmon resonance we have been managed to record the SERS-spectra of Rhodamine 6G at 10^{-6} M concentration upon the excitation with 473, 633 and 785 nm lasers (Fig 1(C)).

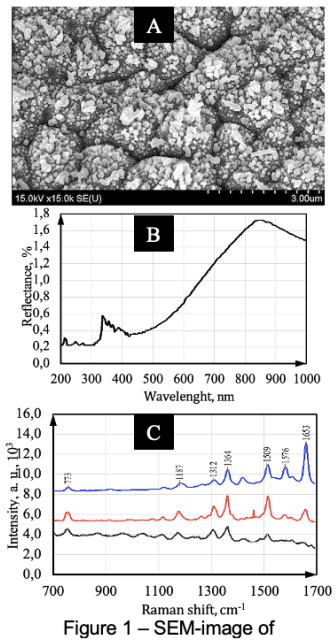

Figure 1 – SEM-image of Ag/Ni/macroPS surface (A), reflectance spectrum (B) and SERS-spectra of Rhodamine 6G 10^{-6} M

The research was supported by BRFFR and RFBR (projects №T21PM-136, №20-58-04016)

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P14. Local electrophoretic deposition of TiO_2-CuO_x nanocomposites for gas sensors

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Today, there is an increased demand for reliable, highly selective portable gas sensors for various applications. Sensitive layers based on semiconductor metal oxides are most relevant due to their high sensitivity to a wide range of oxidizing and reducing gases. Forming a sensing layer in local areas is an important task for reducing the size of sensors and developing multisensor systems. The electrophoretic deposition technology allows to form composites of multicomponent composition in the local area, including complex topological patterns. This paper presents the results of electrophoretic deposition of a TiO_2-CuO_x composite on patterned electrodes.

The electrophoretic deposition was performed from a suspension based on isopropyl alcohol, acetone, the TiO_2 nanopowder, SLS and CuO_x nanopowder in different weight ratios. Sitall substrate covered with Ni layer by magnetron sputtering were used as a substrate. The topological pattern of the electrodes was formed using a laser CNC machine. The distance between the electrodes was 100 μm. The surface morphology, thickness, and stoichiometry of the obtained samples were studied by scanning electronic microscopy and energy dispersive X-ray analysis.

Precise control capability of TiO_2-CuO_x nanocomposites composition by changing the suspension content was demonstrated. The possibility of local deposition of nanocomposites on an electrically conductive topological pattern was shown. The optimal mode of the electrophoretic deposition process for filling the gap between the electrodes was determined.

This work was supported by the Russian Innovation Promotion Fund (UMNIK- 0062117)

P15. Influence of swift heavy Ag^{7+} ion irradiation on room temperature ferroelectric triglycine sulphate single crystal

V.C. Bharath Sabarish[1]*, G. Ramesh Kumar[1], A. Durairajan[2], M. P. F. Graça[2], M.A. Valente[2], S. Gokul Raj[3]

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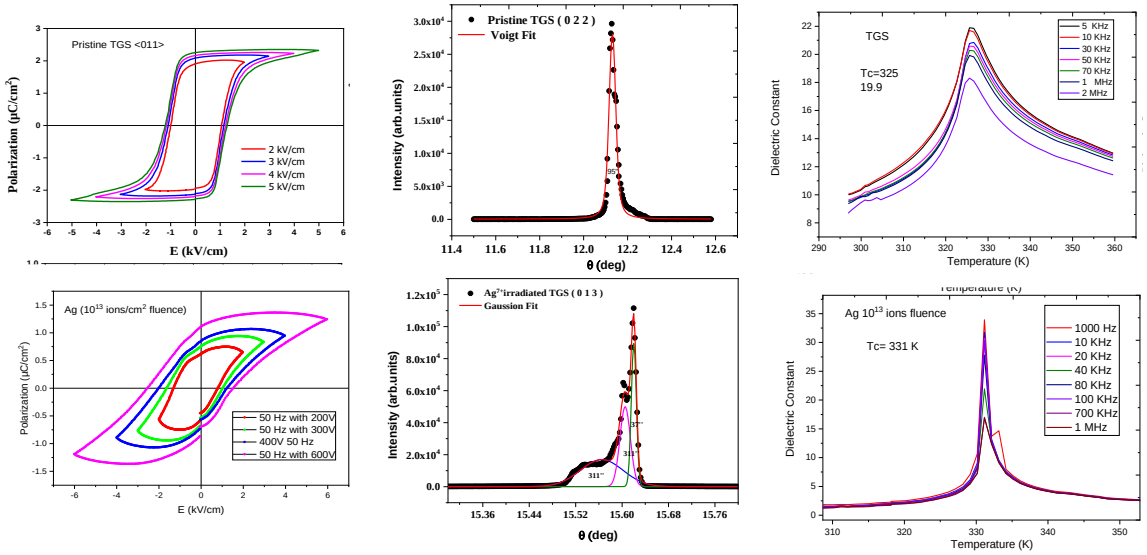
A study on the effect of ferroelectric properties upon irradiating Ag^{7+} (100 MeV) Swift Heavy Ions (SHI) on room temperature TGS single crystals has been made at different fluencies. HRXRD reveals the fact that there is formation of structural defects upon high energy ion impact. Increase in the optical absorption properties of irradiated crystals suggest the creation of defect density, possible defects band transitions occur nearby to the band edge of TGS. The changes in the coercive filed indicate that there are drastic changes in the ferroelectric domain. The other interesting results would be discussed during conference meeting.



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P16. Effect of calcination temperature on vibrational and optical absorption properties of $BiFeO_3$ –Graphene and $BiFeO_3$ –MWCNT nanocomposites

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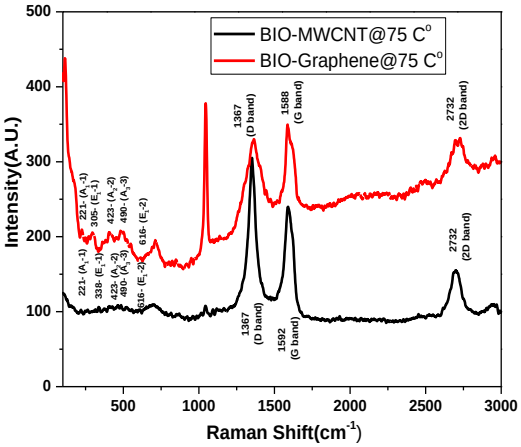
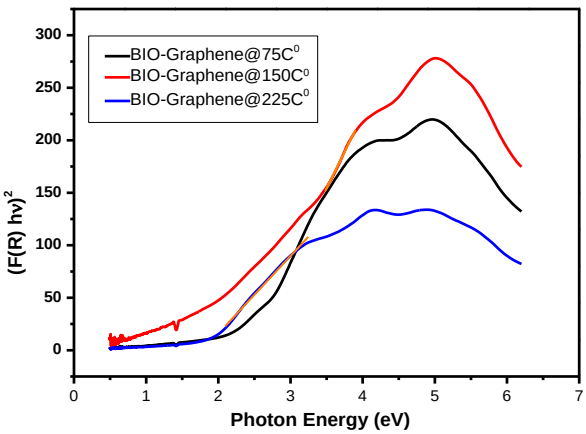
Nanocomposites of $BiFeO_3$ (BFO) with MWCNT and Graphene have been synthesised from sol-gel technique followed by calcination at different temperatures viz 75, 150 and 225˚C. The composite nature of calcinated powders have been characterized using powder XRD, FTIR, UV, Dielectric and Raman analyses. It was observed that optical band found to be decreasing with increase in calcination temperature due to increased defect density of states. In Raman analysis $BiFeO_3$ (BFO) A_1 & E modes and carbonaceous materials bands of (D-band), (G-band) and (2D-band) are present calcined samples of which indicates that particles are highly intercalated. The other interesting results would be discussed in conferences.





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P17. Temperature evolution of the crystal structure and piezoelectric response in $BiFeO_3$-$BaTiO_3$ solid solutions on the rhombohedral-pseudocubic phase boundary

A.S. Abramov[1,*], D.O. Alikin[1], A.P. Turygin[1], A. Zheludkevich[2], D. Zheludkevich[2], A. Pakalniškis[3], R. Skaudžius[3], A.L. Kholkin[1,4], D. Karpinsky[2]

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Bismuth ferrite ($BiFeO_3$) is one of the most perspective multiferroic material with high spontaneous polarization in the thin film form and antiferromagnetism. In the form of ceramics, BFO is extremely difficult to stabilize in the pure defect-free perovskite phase. Both defects and secondary phases are responsible for the high leakage current, impeding achievement of the possible high polarization and piezoresponse. In this contribution, (1-x)$BiFeO_3$-(x)$BaTiO_3$ solid solution was prepared using solid-phase and sol-gel synthesis.

The crystal structure and functional properties of the ceramics were studied at the rhombohedral-pseudocubic phase boundary ($0.2<x<0.4$) in dependence on the temperate. Both X-ray diffraction measurements and dielectric spectroscopy reveal phase transition in the 100°C-200°C temperature range associated with the ferroelectric-relaxor transformation. The visualization of the piezoresponse distribution in the ceramic grains approved the relaxor material state. Notably, a significant enhancement of the piezoresponse was achieved in the relaxor state, followed by the larger rhombohedral distortion of the crystal lattice. As such possibility of the chemical control of the relaxor state in the (1-x)$BiFeO_3$-(x)$BaTiO_3$ solid solution was shown, which looks attractive for future application in the different electromechanical devices.

The study was funded by RFBR (grant No. 19-52-04015) and BRFFR (grant No. F19RM-008). This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020 & UIDP/50011/2020, financed by national funds through the Portuguese Foundation for Science and Technology/MCTES. This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 778070.

P18. Investigation of the optimal method for applying the analyte R6G to the SERS substrate based on silver nanoparticles

N. Mineeva[1, *], S. Dubkov[1], A. Savitsky[1], K. Girel[2], A. Burko[2], S. Zavatsky[2], D. Novikov[1], A.Tarasov[1]

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The aim of this work is to test the effect of the methods of applying aqueous and alcoholic solutions of rhodamine 6G on SERS substrates based on Ag NPs. For the experiments, solutions of R6G with micro-, milli- and nanomolar concentrations based on water and isopropyl alcohol were prepared. Dionized water was used to prepare the aqueous solution; for the alcohol solution, 99.8% isopropyl alcohol was used. Drop dosing and soaking methods were used to apply the analyte to the SERS substrate. The drop dosing method consisted of applying a drop of the analyte using an EKOCHEM dispenser and subsequent drying of the samples in a fume hood at room temperature for 30 minutes. The volume of the applied analyte was about 4 μL. In the soaking method, the prepared SERS substrates were immersed in an analyte solution of the appropriate concentration for 20 minutes. Then it was washed in dionized water and dried in a fume hood at room temperature for 30 minutes. The studies were carried out on a LabRAM HR Evolution Raman spectrometer at wavelengths of 514 and 633 nm.

It was found that the best spectroscopic result is achieved by soaking the substrate in an alcohol solution of R6G. The amplification factor is of the order of 10^5. The dosed drop method has demonstrated the amplification factor of both types of solutions in the range of 10^4. The method of soaking in an aqueous solution showed an amplification factor of about 10^3.

According to the results of the work, the method of soaking an alcohol solution of R6G demonstrates the highest efficiency. However, taking into account the luminescence of this substance in the presence of organic solvents, the dosed drop method is more promising, which provides similar results when using different solutions.

The research was supported by BRFFR and RFBR (projects #T21PM-136, #20-58-04016).

P19. Detection of trimethylamine oxide by surface enhanced raman spectroscopy

D.Novikov[1, *], H.Bandarenka[2], A.Burko[2], S.Zavatsky[2], K. Girel[2], S.Dubkov[1], D.Gromov[1], A. Savitsky[1], A.Tarasov[1]

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The purpose of this work is to test the possibility of detecting micromolar concentrations of trimethylamine oxide in human blood plasma using SERS substrates. In this work, the surface-enhanced Raman spectroscopy (SERS) method was used [1]. For research, substrates with the following planar SERS structure were used: Si plate with 300 nm oxide layer; Me reflective layer 100 nm; transparent SiO_2 insulator layer; a layer of disk-shaped Me nanoparticles with an average diameter of ~ 40 nm. Ag and Au were used as Me. The analytes were aqueous solutions of TMAO micro, mile, and normal concentration, and blood plasma of two different people. The application of the samples to the substrate was carried out with a 4 mcl measuring pipette. The studies were carried out on a LabRAM HR Evolution Raman spectrometer at wavelengths of 514 and 633 nm, with a laser power from 0.005 to 0.5 mW, and x100 focus lens. An additional step was polarization drying in a fume hood with a constant electric field of 50 V and an interelectrode distance of 2 cm. To process the obtained spectra, the KnowItAll Academic Edition program was used. The results of the work showed that to study TMAO-containing solutions, Si/Ag/SiO_2/Ag NPs substrates, lasers with a wavelength of 514 nm and a power of no more than 0.25 mW should be used. Drying the analyte in the presence of an electric field made it possible to increase the intensity of a number of TMAO peaks by 6 times. Studies of blood plasma made it possible to establish an excess of TMAO levels by 1.6 times in person 2 in comparison with person 1. It follows from the work that the SERS substrates can be used to determine the level of TMAO in human blood. To determine the concentration, you must have at least one sample with a predetermined content of TMAO. The work was supported by the Russian Science Foundation (Project No. 21-19-00761).

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P20. Conversions of CO_2 and CH_3OH on the TiO_2 surface under ultraviolet radiation and high pressure

S. Dubkov[1], **A. Overchenko[1*]**, L. Sorokina[1], D. Gromov[1], A. Tarasov[1], T.Maniecki[2], A.Shtyka[2], R. Ciesielski[2]

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Photocatalysis is an efficient cleaning method. Today TiO_2 is a required material, which is used for disinfection of surfaces, air and water. However, due to the peculiarities of the TiO_2 band structure, this material exhibits its photocatalytic properties only when it exposed by the UV radiation, which makes it possible to use only about 4% of the intensity of sunlight radiation. Because of this reason, the development of materials based on the TiO_2 with more efficient use of the visible range of electromagnetic radiation is an urgent task. This problem can be partially solved by using such material like: Ag, Au and Cu. But in order to understand the influence of various factors on titanium dioxide, it is necessary to clearly analyze all the transformations that are observed on TiO_2 during the reaction with organic compounds under different factors such as high pressure.

In the course of this work, the influence of high pressure and different temperatures on modified TiO_2 and the effect of Eu on properties of TiO_2 were studied. Different modifications of TiO_2 were made by impregnation method. To describe the transformations on the TiO_2 surface, an IR Fourier spectrometer used.

It was found that hat under pressure, the reaction rate on the surface will be higher, respectively, and the product size will also be higher compared to standard pressure. The addition of Eu has a positive effect on the amount of adsorption of TiO_2.

The work was supported by the Russian Science Foundation (Project No. 19-19-00595).

P21. Development of approaches to the formation of TiO_2 nanowires for sensitive elements of biosensors

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Biosensors are an attractive object of research due to their high sensitivity and high detection rate. The structure of a biosensor based on a field effect transistor can detect many organic substances such as antibodies, dyes, etc [1]. A semiconductor material made in the form of a one-dimensional object acts as a sensitive element in such sensors. The use of one-dimensional nano-objects opens up new possibilities for creating biosensors with a lower sensitivity threshold, which makes it possible to detect nano- and picomolar concentrations of substances, up to single molecules with different molecular weights.

One of the promising materials used as a sensitive element of a sensor is TiO_2 in the form of nanowires. In nanowires, in comparison with films, there is no depletion and accumulation of charge carriers on the surface and in the bulk of the structure, which contributes to the detection of a small amount of matter [2]. The development of approaches to the reproducible and controlled formation of TiO_2 nanowires is one of the urgent tasks.

In this work, a technique for the hydrothermal synthesis of TiO_2 nanowires is presented and the kinetics of the growth of one-dimensional structures is established. The effect of the annealing temperature on the crystal structure of the obtained samples of TiO_2 nanowires has been studied. The samples obtained were examined using SEM, X-ray structural analysis and Raman spectroscopy.

This work was financially supported by the grant of President of the Russian Federation (project МК-2201.2021.4).

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Workshop on Low-dimensional materials: experiment, theory, application

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Workshop program

July 6, 2021

9:15-10:15
The growth- and coalescence behaviour of graphene: Insights from in-situ scanning electron microcopy
Prof. Dr. Marc Georg Willinger
ETH Zurich, Department of Materials, Scientific Center for Optical and Electron Microscopy, Zurich, Schweiz

10:45–11:15
2D- Photocatalyst: 6, 13- Pentacenequinone (PQ) for Future
Prof. Dr. Vikram Uttam Pandit
Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India

11:15–12:00
Modeling of Low-dimensional & 2D-materials
Prof. Dr. Vladimir Bystrov
Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia

12:00–12:30
Two Dimensional Zinc Oxide (2D-ZnO) Nanostructures for MB Dye Degradation
Prof. Dr. Vikram Uttam Pandit / VIVEKANAND JAWALE
Haribhai V. Desai Arts, Science & Commerce College, Pune-411002, India

14:00–14:45
Graphene-based nanocomposites with high-performance for health and environmental applications
Dr. Gil Gonçalves
TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal

14:45–15:15
Free Vibration Analysis of rotating Single Walled Carbon Nanotubes Resting in Elastic Medium
Prof. Dr. Abdelkadir Belhadj
DC Engineering & Project Management, Sonatrach, Algiers, Algeria; Computational Mechanics Laboratory, Faculty of Technology, University of Tlemcen, Tlemcen, Algeria

15:15–15:45
Low-dimensional effects in Atomic Force Microscopy (AFM)
Dr. Igor Bdikin
TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal

Plenary lecture

W-PL1. The growth- and coalescence behaviour of graphene: Insights from in-situ scanning electron microcopy

Marc Willinger

Scientific Center for Optical and Electron Microscopy, ScopeM, ETH Zürich, 8093 Zürich, Switzerland

We have modified the set-up of a conventional scanning electron microscope (SEM) in order to enable the observation of catalyst surface dynamics under controlled atmosphere and temperature. Using this instrument, we have performed *in situ* investigations on chemical vapor deposition (CVD) growth of graphene on different metal catalysts. Since our growth studies are performed in the chamber of a microscope, it is possible to observe complete CVD processes starting from substrate annealing through graphene nucleation and growth and, finally, substrate cooling in real time at nanometer-scale resolution without the need of sample transfer. The nucleation and growth of single layer graphene can be investigated at temperatures of up to 1000°C, while at the same time, surface dynamics of the active metal catalyst can be studied. Growth on polycrystalline substrates reveals grain orientation dependent growth dynamics and catalytic activity [1,2]. Due to the high sensitivity of the secondary electron signal to changes in the work function and charge transfer at the surface, we are able to visualize different degrees of graphene-substrate coupling [3]. Real-time imaging under well-controlled atmosphere furthermore enables combined growth- and etching experiments and thus, studies on the stacking sequence and interlayer coupling strength in few-layer graphene [4,5] More recently, we have investigated the effect of the film-substrate interaction strength on the coalescence behavior of graphene. Based on our observations, we were able to define criteria for seamless coalescence of graphene islands [5]. As will be shown, the findings revealed by direct real-time observation are important for the industrial production of large area single-crystalline graphene flakes.

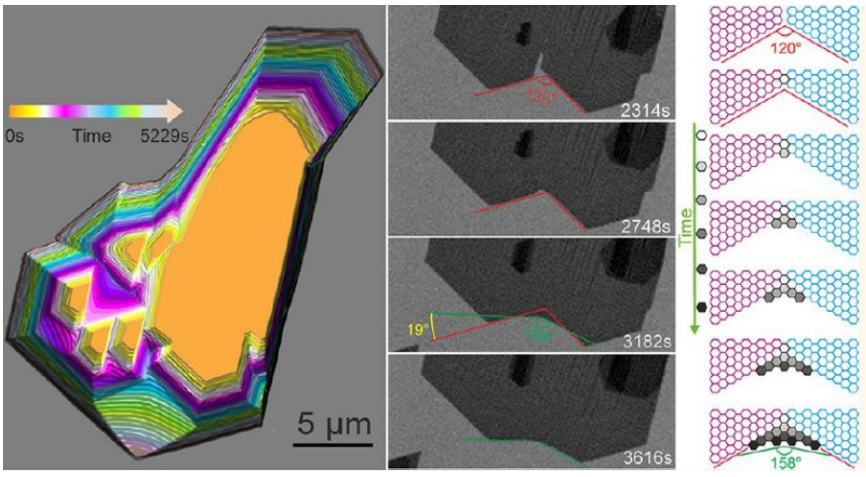

Figure 1: Although the scanning electron microscope does not provide in-plane atomic resolution, it is possible to abstract atomistic details about the coalescence behaviour of graphene islands: Analysis of the temporal evolution reveals the underlying processes that lead to the formation of fast growing growth-fronts in seamless coalescence.

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Plenary lecture

W-PL2. Modeling of Low-dimensional & 2D-materials

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The development of modern computational methods allows us to model, calculate and predict the structure and properties of a wide range of nanomaterials, including nanoscale and low-dimensional materials. Particular interests are two-dimensional (2D) nanomaterials, such as, for example, dichalcogenides of transition metals (DCTM: type MoS_2 and similar), graphene and materials based on graphene/ graphene oxide, ultrathin ferroelectric Langmuir-Blodgett polymer films (like PVDF and P (VDF -TrFE)) and also their various hybrid heterostructures and composites. These promising materials have many uses: sensors and sensors, nanogenerators and transducers, memory elements, photodetectors and photocatalysts, etc.

Existing computational methods based on standard local and semilocal approximations in density functional theory (DFT) play an important role in understanding the structure and electronic, optical, electrical and magnetic properties of these materials. As well as ab initio and semi-empirical quantum mechanical methods (AM1, PM3, PM6, RM1 etc.). However, unfortunately, these approaches, as well as DFT approaches based on local functionals, do not always provide sufficient accuracy. Therefore, there is a constant development of methods, it becomes necessary to use methods of a higher level, such as nonlocal functionals, the application of the Green's function methods, the random phase approximation or the methods of many-body perturbation theory. At the same time, the methods of classical molecular mechanics with well-developed force fields (Amber, BIO CHARM, etc.) are often sufficient to identify some basic regularities and properties of 2D materials. Moreover, the most effective here can be combined methods that combine the approaches of both classical MM and quantum QM, and of different level. Here it is necessary to take into account their correct combination at various stages of modeling/calculations. As examples here we are considering:

1) nanoscale 2D-ferroelectric films based on PVDF, the kinetics of polarization switching in these films and the influence of the implement graphene layers on these processes (using molecular dynamics simulation with quantum PM3 RHF calculations at each step in the HyperChem software framework);

2) layered structures of MoS_2 dichalcogenides by DFT methods in the generalized gradient approximation with the PBE functional and taking into account the van der Waals interactions as PBE + D3 in the VASP and Quantum ESPRESSO programs;

3) hybrid hetero-structure based on “MoS_2 + PVDF” using the combined DFT and semi-empirical PM3 RHF methods.

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Plenary lecture

W-PL3. Graphene-based nanocomposites with high-performance for health and environmental applications

Gil Gonçalves

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Carbon is one of the most relevant elements on the earth to all forms of life and presenting a wide range of natural allotropic forms with high economic potential. Inspired by nature, scientists started to design synthetic strategies for the development of novel allotropic carbon nanomaterials. Harry Kroto et al. is considered the pioneer in this field with the discovery of fullerenes in 1985, which culminated with the attribution of the Nobel Prize in Chemistry in 1996. [1] Curiously, recently it was detected evidence of the presence of fullerenes in extraterrestrial environments.[2] Afterward, the graphene groundbreaking experiments constituted a significant mark on the field of carbon nanomaterials, by reporting for the first time the characterization of a 2D crystal with atomic thickness under natural conditions [3], which resulted in the attribution of the Nobel Prize in Physics in 2010. This remarkable achievement created a new highway in the research field of two-dimensional materials. [4] The versatility of carbon atoms on the establishment of different chemical interactions between themselves and many other elements has been allowed the development of novel nanostructured materials with improved performance. The recent advances in the research of carbon nanomaterials have led to the development of new exciting nanocomposites able to address several societal challenges. Here, I will present my current research on the design of novel carbon-based nanocomposite and provide my vision on their application in the exciting and fast-growing field of biomedicine [5] and environment [6].

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Invited talk

W-I1. Free vibration analysis of rotating single walled carbon nanotubes resting in elastic medium

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Many significant researches in nanomechanics have been conducted to develop new nanomaterials using different emerging techniques to understand their behavior. Nanostructures are widely used as nanobeams, nanoplates and nanoshells, nanobeams based single walled carbon nanotubes (SWCNT) are applied as nanosensors, nanoprobes, nanowires, nano-resonators, nano-actuators, material reinforced nanostructure[1-3].

In this paper, a computational structural dynamic analysis based on Eringen's elastic constitutive model is done to investigate the free vibration of SWCNT resting in an elastic medium of Winkler type. First, the theory of non local elasticity is introduced to be applied to the classical Hooken equations, the governing equations to be generated by applying the Hamilton's principles. For solving differential equations system, the generalized differential quadrature method (GDQM) has been chosen to discretize the equations; a new technique for boundary conditions imposition has been used in the Matlab's code, which is developed to solve the following equations:

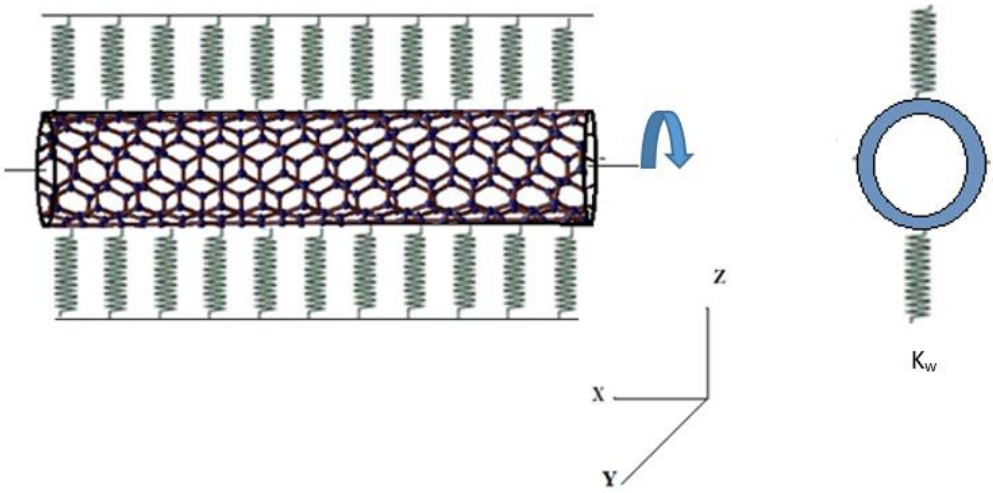
$$-\rho A\omega^2\left(1-(e.a)^2\frac{d^2}{dx^2}\right)u - EA\frac{d^2u}{dx^2} \quad = 0 \tag{1}$$

$$-\rho A_y\omega^2\left(1-(e.a)^2\frac{d^2}{dx^2}\right)v + \rho I\omega.j\left(1-(e.a)^2\frac{d^2}{dx^2}\right)v - 2\Omega\left(1-(e.a)^2\frac{d^2}{dx^2}\right)j\omega w - EI\frac{d^4v}{dx^4} + k\left[w-(e.a)^2\frac{d^2v}{dx^2}\right] = 0 \tag{2}$$

$$-\rho A_z\omega^2\left(1-(e.a)^2\frac{d^2}{dx^2}\right)w + \rho I\omega.j\left(1-(e.a)^2\frac{d^2}{dx^2}\right)w + 2\Omega\left(1-(e.a)^2\frac{d^2}{dx^2}\right)j\omega v - EI\frac{d^4w}{dx^4} + k\left[w-(e.a)^2\frac{d^2w}{dx^2}\right] = 0 \tag{3}$$

By solving the problem, on define the frequency parameter, the angular velocity parameter, and the elastic coefficient parameter. Campbell diagram is elaborated to show the variation of frequency parameter, which is split into forward and backward frequency. The nonlocal parameter has effected the frequency parameters decreasingly.

The effect of the elastic coefficient parameter on the rotation of the small scale structure is discussed in order to understand the behavior of the spinning SWCNT embedded in an elastic medium. Results of this study can serve as good guidance for next generation nano-machines.



A rotating SWCNT resting in an elastic medium.

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Oral presentation

W-O1. 2D-photocatalyst: 6, 13-pentacenequinone (PQ) for future

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Of late, inorganic material based photocatalysis helps to treat industrial waste water up to some extent. Aromatic, complex, organic dyes and pigments are the wastes which damages the human health as well as aquatic life. Researchers are working to overcome this serious issue from many years, but to developed cost-effective and eco-friendly method is unsolved challenge. We have synthesized 6, 13- pentacenequinone (PQ) an intermediate require synthesizing pentacene which is well known organic semiconductor. After complete characterization we explored PQ for industrial dye degradation and photocatalytic H_2S splitting for the first time. We also synthesized composite system of PQ-TiO_2 with inorganic semiconductor photocatalyst. Recently a report of PQ-MoS_2 photocatalyst also covers the water splitting area. This organic PQ photocatalyst have high potential in photocatalysis field which can be utilized for the clean environment and for water treatment.

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Oral presentation

W-O2. Two dimensional zinc oxide (2D-ZnO) nanostructures for MB dye degradation

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The 2D zinc oxide (ZnO) nanostructures were synthesized using hydrothermal reaction technique at 180°C with varying reaction time viz., 2, 4, 8 and 12 h. The prepared ZnO nanostructures were characterized with different spectroscopic and microscopic techniques. The XRD indicate the formation of hexagonal phase of ZnO in all the prepared samples. The UV-visible absorbance spectrum depicts the absorption peak at 380 nm corresponding to the band gap of 3.27 eV. The FESEM confirms the formation of hexagonal shaped plate like ZnO nanostructures having size in the range of 50 to 100 nm with the thickness of 10-15 nm, at 2 h reaction time. The TEM validates the formation of highly crystalline hexagonal shaped ZnO plates having size in the range of 0 to 150 nm. The photocatalytic activities of prepared ZnO nanostructures were investigated by following degradation of 100 mL, 10 ppm methylene blue (MB) dye. Among the prepared ZnO nanostructures, the ZnO prepared at 8 h of reaction time shows highest MB degradation rate, the observed apparent rate constant value is 3.3 x 10^{-2}± 0.1 x 10^{-2} min^{-1}, which is five times more than 4 h reaction time.

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Oral presentation

W-O3. Low-dimensional effects in Atomic Force Microscopy (AFM)

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In the past 20 years, various types of low-dimensional structures have been developed: 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, generators etc. Currently, it is becoming increasingly obvious that develop new methods for investigation of micro- and nano- structures is extremely necessary. So, in case of virus infections (Pandemia COVID-19) one of main problem is rapid detect and characterization of low-dimensional and nanoscale structures. Therefore, methods for detection, visualization, analysis of the microstructures must be in priority nanotechnology. One of this very perspective method is atomic force microscopy (AFM). AFM has achieved great success in single-cell observation, single DNA molecules, organic microstructures and manipulation for biomedical applications, demonstrating the excellent capabilities of AFM in addressing biological issues at the single-macromolecular level with unprecedented spatiotemporal resolution.

Here we show the applicability and current problems of AFM for studying a broad range of low-dimensional materials at the nanoscale for organic and non-organic complex structures: thin films [1,2], nano tubes [3,4], fibers [5], domains [6].

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

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

Notes

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