3rd International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal
July 7-10, 2020

Book of Abstracts

tema university of aveiro
centre for mechanical technology and automation

FCT Fundação para a Ciência e a Tecnologia
CENTRO 2020
PORTUGAL 2020
UNIÃO EUROPEIA
Fundo Europeu de Desenvolvimento Regional

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Editors
Igor Bdikin
Raul Simões

Publisher
UA Editora
Universidade de Aveiro

1st edition – July 2020

ISBN
978-972-789-644-8

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3rd International Conference on Nanomaterials Science and Mechanical Engineering,
2nd Workshop on Characterization and Analysis of Nanomaterials
and
Workshop on Local-scale and magneto-electric measurements in functional nanomaterials
(3rd ICNMSME-2020 / 2nd WCANM-2020)
looks for significant Modern Problems of Nanomaterials Science and Mechanical Engineering, to provide a platform to the global researchers and practitioners from both academia as well as industry to meet and share cutting-edge development in the fields, to give possibility for young scientists and students present results and find your place in the future world.

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Conference Web

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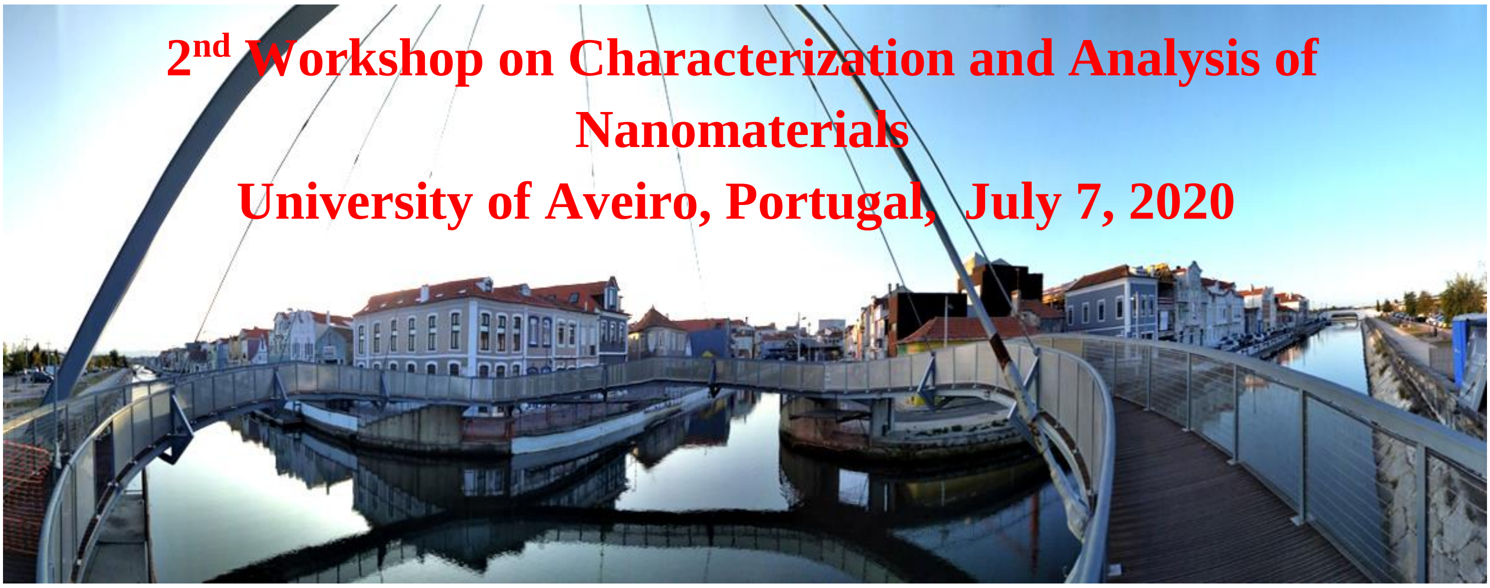
2nd Workshop on Characterization and Analysis of Nanomaterials

University of Aveiro, Portugal, July 7, 2020



Progress in science depends mainly on the level of experimental technology. Currently, interest in nanomaterials has led to many technological advances and has opened new horizons in understanding nature. Success in these ways possible by the development and standardization of methods for determining the characteristics of nanomaterials: X-ray diffraction, electron microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, modelling of nanostructures, etc. A thorough knowledge of these methods is a necessary basis for work in modern science. The major aim of this workshop is to give a detailed description of principles and current state of the basic methods for characterization of nanomaterials.

2nd WCANM-2020 Organizing committee

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2nd Workshop on Characterization and Analysis of Nanomaterials **University of Aveiro, Portugal, July 7, 2020 (*online*)** **Auditorium 1**	
9:00-9:15	**WELCOME ADDRESS** **Prof. Dr. António Manuel de Bastos Pereira, Dr. Igor Bdikin**
9:15-10:15	CHAIR: Dr. Duncan Paul Fagg **X-ray diffraction (XRD)** **Prof. Dr. Dmitry Karpinsky** **National Research University of Electronic Technology, Moscow, Russia** **Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus**
10:15–10:30	**Coffee break / Open discussions**
10:30–11:30	CHAIR: Dr. Igor Bdikin **Modelling of nano-structures** **Prof. Dr. Manuel Melle-Franco** **CICECO, University of Aveiro, 3810-193 Aveiro, Portugal** **1. Computer simulation and multiscale modelling.** **2. How to Use Computer Modelling to Complement Experiments.**
11:30–12:00	**Work in HyperChem tools - modeling and calculations:** **on the example of polymer ferroelectrics like PVDF** **Prof. Dr. Vladimir Bystrov** **Inst. Mathematical Problems of Biology,** **Keldysh Institute of Applied Mathematics RAS,** **Pushchino, Moscow region, Russia**
12:00–13:00	CHAIR: Dr. Gil Gonçalves **Raman Spectroscopy** **Prof. Dr. Helena Isabel Seguro Nogueira** **CICECO, Department of Chemistry, University of Aveiro, Portugal**

13:00–14:00	**Lunch break**
14:00–15:00	CHAIR: Dr. Igor Bdikin **Atomic force microscopy (AFM)** **Dr. Denis Alikin** **School of Natural Sciences and Mathematics,** **Ural Federal University, Ekaterinburg,** **Russia** **Department of Physics & CICECO – Aveiro Institute of Materials,** **University of Aveiro, Aveiro,** **Portugal**
15:00–16:00	CHAIR: Dr. Gonzalo Guillermo Otero **Electron Microscopy** **In-situ Electron Microscopy** **Prof. Dr. Marc Georg Willinger** **Scientific Center for Optical and Electron Microscopy (ScopeM)** **ETH Zürich,** **Switzerland**
16:00–16:30	**Coffee break / Open discussions**
16:30–17:30	CHAIR: Dr. Gonzalo Guillermo Otero **X-ray Photoelectron Spectroscopy (XPS)** **Prof. Dr. Jose Angel Martín Gago** **Institute of Material science of Madrid-CSIC,** **Madrid,** **Spain**
17:30–17:45	**Final discussions and comments**

8 July 2020

3rd International Conference on Nanomaterials Science and Mechanical Engineering (*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- 10:15	Session: **New Materials and Advanced Materials** CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques, Prof. Dr. António Manuel de Bastos Pereira ***Plenary Lecture*** Prof. Dr. Marc Georg Willinger **Spatio-temporal dynamics of active catalysts observed by multi-scale in-situ electron microscopy** *Scientific Center of Optical and Electron Microscopy, ScopeM, ETH Zürich, Otto-Stern-Weg 3, 8093 Zürich, Switzerland*		
10:15- 11:00	***Plenary Lecture*** Prof. Dr. Anatoly Dvurechenskii **Site-controlled Nucleation in Ordered Array of Epitaxial SiGe Quantum Dots: Growth, Properties and Application** *Rzhanov Institute of Semiconductor Physics, Novosibirsk, Russia*		
11:00- 11:30	Coffee break		
	Auditorium 1 Session: **Nanotechnology** CHAIR: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques	**Auditorium 2** Session: **Micro / Nano Materials** CHAIR: Dr. Denis Alikin	**Auditorium 3** Session: **Protective Coatings and Corrosion of Materials** CHAIR: Prof. Dr. Neeraj Panwar
11:30- 12:00	***Keynote talk*** Prof. Dr. Dmitry Karpinsky (**I3**) **Structure and magnetic properties of Sm doped BiFeO3 ceramics across the rhombohedral-orthorhombic phase transition** *Cientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus*	***Keynote talk*** Prof. Dr. Radheshyam Rai (**I14**) **Negative dielectric permittivity material based on La and Pr doped EuMnO3 perovskite system** *Eternal Univ, Dept Phys, Akal Coll Basic Sci, Sirmour, Himachal Prades, India*	***Keynote talk*** Dr. Kiryl Yasakau (**I13**) **Localized corrosion at zinc-galvanized surface and corrosion prevention strategies** *University of Aveiro, Portugal*

12:00-12:30	Dr. J. Nischal Kiran (**O8**) **Synthesis, Structural, Tribological and Magnetic characterization of Double doped Strontium Bismuth Niobate Lead free ceramics** *Department of S&H, VFSTR deemed to be University, Vadlamudi, Guntur – 522002, India*	Dimitra Das (**O3**) **Reduction of Toxic Pollutants from Water Environment by Rod-like Silver Coordinated Melamine based Polymer** *School of Materials Science and Nanotechnology, Jadavpur University, Kolkata, India*	Mohamed el Messoudi (**O9**) **Flame retardant finishing of cotton fabric based on Ionic liquid compounds containing boron prepared with the sol-gel method** *Laboratory REMTEX, ESITH (Higher School of textile and clothing industries), Casablanca, Morocco*
12:30-13:00	Dr. Avesh Kumar (**O23**) **Tunable efficiency of Au-TiO2 nanocomposites** *Physical Research Laboratory, Ahmedabad-380009, India*	Dr. Mihaela Beregoi (**O25**) **Electroactive materials based on polypyrrole coated electrospun nanofibers** *University Politehnica of Bucharest, Faculty of Applied Chemistry and Materials Science, Bucharest, Romania*	Session: **Nanotechnology** CHAIR: Prof. Dr. Neeraj Panwar Ivana Katarina Munda (**O26**) **Characterization of sol-gel-derived ceria nanoparticles doped with manganese** *University of Zagreb, Faculty of Chemical Engineering and Technology, Zagreb, Croatia*
13:00-14:00	Lunch		
14:00-14:45	**Auditorium 1** Session: **Low Dimension Structures** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta Dr. Igor Bdikin ***Plenary Lecture*** Prof. Dr. Jose Angel Martín Gago **Graphene: From fundamental research to technological applications** *Institute of Material science of Madrid-CSIC, Madrid, Spain*		
14:45-15:30	Session: **New Methods of Modeling Properties Materials** CHAIRS: Dr. Gonzalo Guillermo Otero Irurueta Dr. Igor Bdikin ***Plenary Lecture*** Prof. Dr. Vladimir Bystrov **Computer modeling and calculations of the physical properties of self-assembled nanostructures & nanotubes based on various amino acids (a review)** *Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*		
15:30-16:00	Coffee break		

	Auditorium 1 Session: **New Materials and Advanced Materials** CHAIR: Dr. Gonzalo Guillermo Otero Irurueta	**Auditorium 2** Session: **New Methods of Modeling Properties Materials** CHAIR: Dr. Gil Gonçalves	**Auditorium 3** Session: **Micro / Nano Materials** CHAIR: Prof. Dr. Dmitry Karpinsky
16:00-16:30	***Keynote talk*** Prof. Dr. Neeraj Panwar (**I9**) **Manganese substitution effect on the structural, optical, magnetic and magnetocaloric properties of HoCrO3 orthochromite** *Department of Physics, School of Physical Sciences, Central University of Rajasthan, Bandarsindri-305817, Ajmer, Rajasthan-INDIA*	***Keynote talk*** Dr. Karine Abgaryan (**I23**) **Multiscale modeling of multilevel memory elements as synapses necessary for creating neuromorphic networks** *Federal Research Center "Computer Science and Control" of the Russian Academy of Sciences (FRCCSC) Vavilov st. 40, 119333 Moscow, Russia*	***Keynote talk*** Prof. Dr. Vijay Raj Singh (**I27**) **Effect of Disorder on the Metal-Insulator Transition of Vanadium Oxides by Soft X-Ray Irradiation** *Department of Physics, Boston University, Boston, MA 02215, USA*
16:30-17:00	***Keynote talk*** Dr. Ranjit Hawaldar (**I24**) **Growth of Few layered 2D materials by Chemical Vapor Deposition** *Centre for Materials for Electronics Technology, Pune, India*	***Keynote talk*** Dr. Manuel Melle-Franco (**I19**) **Computer Simulations: the Ultimate Tool to Understand Nanotechnology Experiments** *CICECO, Department of Chemistry, University of Aveiro, 3810-193,Aveiro, Portugal*	***Keynote talk*** Dr. Pankaj Bharmoria (**I17**) **Protein based Biomaterials from Biocatalysis to Photonics** *Kasper Moth-Poulsen Lab, Department of Applied Chemistry, Chalmers University of Technology, Kemivägen 4, 412 96 Gothenburg, Sweden*
17:00-17:30	Sarka Sovova (**O18**) **Temperature and time controlled synthesis of instable vaterite microparticles** *Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkynova 464/118, 612 00, Brno, Czech Republic*	***Keynote talk*** Dr. José Coutinho (**I15**) **Modeling electrons in solids, surfaces and nanostructures (with an introduction to density functional methods)** *I3N & Department of Physics, University of Aveiro, Campus Santiago, 3810-193, Portugal*	Dr. Huan Doan (**O24**) **Novel hierarchical copper-based metal-organic frameworks for improved catalytic performance** *Department of Mechanical Engineering, University of Bristol, Bristol BS8 1TH, UK*

17:30- 18:00	Vanessa C.D. Graça (**O41**) **Niobium nitride as electrocatalyst for ammonia synthesis: synthesis and stability conditions** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*	***Keynote talk*** Prof. Dr. Jamal Davoodi (**O31**) **Mechanical properties of Twin Graphene Nanotubes: A molecular dynamics simulation** *Department of Physics, Faculty of Science, University of Zanjan, Zanjan, Iran*	Dr. Victor Krayzman (**O35**) **Whole-particle models of atomic arrangements in brookite titania nanorods** *Materials Measurement Science Division, National Institute of Standards and Technology, Gaithersburg MD 20899, USA*
18:00- 18:30	Laura Holz (**O39**) **The influence of ammonolysis temperature on physical properties of vanadium oxynitride (VOxN1-x) solid solutions** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Portugal*	Sujith Reddy Varakantham (**O32**) **Simulation of interacting and non-interacting dipolar systems and their temperature dependencies** *Institute of Electrical Engineering Physics, Saarland University, Germany*	Katarina Mužina (**O27**) **Synthesis and characterization of copper doped ceria nanocatalyst** *Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10 000 Zagreb, Croatia*
18:30- 19:00	***Keynote talk*** Prof. Dr. Dmitry A Kiselev (**I5**) **The effect of synthesis temperature on the microstructure and electrophysical properties of multifunctional BST thin films** *National University of Science and Technology MISIS, Department of the Material Science of Semiconductors and Dielectrics, Moscow, Russia*	***Keynote talk*** Prof. Dr. Budhendra Singh (**I8**) **Structural, Optical and Mechanical property of pure and Sulphur doped Gallium Selenide: A first Principle study** *Department of Physics, Central University of South Bihar, Gaya, India*	Session: **Nanotechnology** CHAIR: Prof. Dr. Dmitry Karpinsky ***Keynote talk*** Dr. Venkata Ramana Eskilla (**I25**) **Fabrication of BCZT piezoelectrics for energy conversion** *3N-Aveiro, Department of Physics, University of Aveiro, Aveiro 3810 193, Portugal*

9 July 2020

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Dr. Igor Bdikin
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Prof. Dr. Nikolai Sobolev
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Physics Department & i3N, University of Aveiro, 3810-193 Aveiro, Portugal</td></tr>
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Crystal Lab, Department of Physics & Astrophysics, University of Delhi, India</td></tr>
<tr><td>10:30-
11:00</td><td colspan="2">Coffee break</td></tr>
<tr><td></td><td>Auditorium 1
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CHAIR: Dr. Igor Bdikin</td><td>Auditorium 2
Session: Manufacturing Processes and Mechanical Engineering
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<tr><td>11:00-
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Structure and Luminescent Properties of Cyan emitting Eu2+-doped BaAl2O4 Nanophosphors
School of Materials Science and Nanotechnology, Jadavpur University, Kolkata, India</td><td>Prof. Dr. Boutahari Said (O12)
Statistical tolerance analysis of flexible assembly taking into account spot welding effects
High School of Technology of Fez, University sidi mohamed ben abdellah B.P 2626 –Route d'Imouzzar, 30000 Fez, Morocco</td></tr>
<tr><td>11:30-
12:00</td><td>Keynote talk
Dr. Andrei Kovalevsky (I11)
Strontium titanate and zinc-oxide-based materials for high-temperature thermoelectric harvesting
CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal</td><td>Dr. Atik Hafsa (O16)
Tolerance analysis of mechatronics systems
ITS laboratory, High School of Technology, Sidi Mohamed Ben Abdellah University, Morocco</td></tr>
</table>

12:00- 12:30	***Keynote talk*** Dr. Denis Alikin (**I20**) **Chemical Solution Deposition of BiFeO3 Films with Layer-by-Layer Control of the Coverage and Composition** *Department of Physics & CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal*	Wallyson Thomas (**O30**) **Comparison Between The Performances Of Different Boring Bars In The Internal Turning Of Long Overhangs** *University of Miskolc, Miskolc, 3515 - Hungary*
12:30- 13:00	Arushi Gupta (**O15**) **Amino terephthalic Acid Functionalized Graphene Electrode For Impedimetric Immunosensing Of E. coli** *CSIR-Central Scientific Instruments Organisation (CSIR-CSIO), Sector 30 C, Chandigarh, India*	Miguel Fernandes (**O34**) **CFRP Use in SLV Propellant Tanks - Concept and FEM Study** *Aerospace Sciences Department, University of Beira Interior. Convento de Sto. António. 6201-001 Covilhã. Portugal*
13:00- 14:00	Lunch	
14:00- 14:45	**Auditorium 1** Session: **Mechanical Engineering** CHAIRS: Dr. Gil Gonçalves, Dr. D. Pukazhselvan ***Plenary Lecture*** Prof. Dr. Ezddin Hutli **Measurements for Verification and Validation of a Thermal-Hydraulic Computer Code Used for Thermal-hydraulic Analysis of a Complex Flow Geometry Field** *Centre for Energy Research MTAEK. Budapest University of Technology and Economics (BME)- Institute of Nuclear Techniques (NTI). University of Belgrade - Faculty of Mechanical Engineering. Budapest University of Technology and Economics (BME)- Department of Electronics Technology, Budapest, Hungary*	
	Auditorium 1 Session: **New Materials and Advanced Materials** CHAIR: Dr. Gil Gonçalves	**Auditorium 2** Session: **Nanotechnology** CHAIR: Dr. D. Pukazhselvan
14:45- 15:15	Vipasha Sharma (**O29**) **Graphene Quantum Dot Modified Screen Printed Carbon Electrodes for Cortisol Sensing** *CSIR- Central Scientific Instruments Organisation, Sector -30 C, Chandigarh, 160030, India*	***Keynote talk*** Dr. Elena Borisenko (**I22**) **GaTe melt grown single crystals for optoelectronics: solid state phase transitions, structural defects, optical propertries** *Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, Moscow District, Russia*

15:15-15:45	Session: **Biomaterials** CHAIR: Dr. Gil Gonçalves Jayanta Sarmah Boruah (**O4**) **Carbon nanoparticle-vesicles nanocomposites for biomedical applications** *Material Nanochemistry Laboratory, Physical Sciences Division, Institute of Advanced Study in Science and Technology, Paschim Boragaon, Garchuk, Guwahati-781035, India*	***Keynote talk*** Prof. Dr. Sergey Bozhko (**I4**) **Nanoscale inhomogeneity in oxide single crystals: NiO and Ni1-xLixO case** *Institute of Solid State Physics RAS, Russia*
15:45-16:15	Session: **Sensor Materials, Biomaterials** CHAIR: Dr. Gil Gonçalves ***Keynote talk*** Prof. Dr. Helena Isabel Seguro Nogueira (**I18**) **Raman Imaging in SERS Studies** *CICECO, Department of Chemistry, University of Aveiro, 3810-193,Aveiro, Portugal*	Dr. Igor Bdikin (**O44**) **Piezoresponse force microscopy of organic materials** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*
16:15-16:45	***Keynote talk*** Prof. Dr. Cicero R. Cena (**I16**) **Alternative strategies for biosensing studies: Optical spectroscopy and Multivariated Analysis** *UFMS – Universidade Federal do Mato Grosso do Sul, Campo Grande-MS, Brasil*	***Keynote talk*** Prof. Dr. Maxim Silibin (**I2**) **Magnetic properties of (1-x)BiFeO3 – xBaTiO3 ceramics across the phase boundary** *National Research University of Electronic Technology, Moscow, Russia*

Evening Poster Sessions

	Auditorium 1	**Auditorium 2**	**Auditorium 3**
16:45-18:45	CHAIR: Dr. Gil Gonçalves **P1-P13**	CHAIR: Dr. Igor Bdikin **P14-P27**	CHAIR: Dr. Andrei Kovalevsky **P28-P41**

10 July 2020

3rd International Conference on Nanomaterials Science and Mechanical engineering *(online)*

	Auditorium 1	**Auditorium 2**
	Session: **Thin Films, Low Dimension Structures** CHAIR: Dr. Kiryl Yasakau	Session: **Biomaterials** CHAIR: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques
9:00-9:30	Vsevolod Mararov (**O5**) **Adsorption of C60 fullerenes on metal-modified Si(111) surfaces** *Institute of Automation and Control Processes Far Eastern Branch of the Russian Academy of Sciences (IACP FEB RAS) 5, Radio st., Vladivostok, 690041, Russia*	***Keynote talk*** Dr. Svitlana Kopyl (**I1**) **Self-assembled diphenylalanine microtubes: structure, characterization and application** *Department of Physics & CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal*
9:30-10:00	Session: **New Energy Materials** CHAIR: Dr. Kiryl Yasakau Mewin Vincent (**O43**) **Cobalt decorated TiO2 nanosheet as high pseudocapacitance cathode for long lasting rechargeable Mg-Li hybrid batteries** *Faculty of Science, Autonomous University of Madrid, C/Francisco Tomás y Valiente 7, 28049, Madrid, Spain; Electrochemistry Division, IMDEA Materials Institute, C/Eric Kandel 2, Getafe, 28906, Madrid, Spain*	Dr. K. Sowri Babu (**O11**) **ZnO-nanorods grown on flexible substrate for selective host peripheral blood mononuclear cells immobilization** *Division of Physics, Dept. Of Science and Humanities, Vignan's Foundation forScience, Technology & Research (Deemed to be University), Vadlamudi 522213, Guntur, AP, India*
10:00-10:30	Coffee break / Morning Poster Session (CHAIR: Dr. Igor Bdikin)	
	Session: **Thin Films** CHAIR: Dr. Kiryl Yasakau	Session: **Environmental Friendly Materials, Composites** CHAIR: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques
10:30-11:00	***Keynote talk*** Dr. Peter Mozhaev (**I7**) **Graphoepitaxial 3DGE growth of multilayer thin film heterostructures** *Institute of Physics and Technology, Moscow, Russia*	Prof. Dr. Małgorzata Franus (**O6**) **Properties of lightweight aggregates obtained from clay and spent zeolitic adsorbents** *Lublin University of Technology, Faculty of Civil Engineering and Architecture, Department of Construction, Lublin, Poland*

11:00- 11:30	Priyanshu Goel (**O2**) **Metal Halide Perovskite Nanomaterial and MOF Composite Thin Film electrode fabrication using commercially available inkjet printer** *Central Scientific Instruments Organization (CSIR-CSIO), Sector 30 C, Chandigarh,160030, India*	Vishal Shrivastav (**O22**) **UiO-66 Derived Novel ZrO2/C Composite For 2V ElectrochemicalCapacitor: An Approach to Conductive Additive Free Electrode Material** *CSIR-Central Scientific Instrument Organisation (CSIR-CSIO), Chandigarh 160030, India*
11:30- 12:00	Dmytro Rumiantsev (**O33**) **Mesoscopic self-ordering in the (2×1) cerium-molybdenum(112) nanostructures** *Institute of Physics, Natl. Acad. of Sci. of Ukraine, Nauki ave., 46, Kyiv 03680, Ukraine*	Dr. Shashank Sundriyal (**O21**) **A 1.6 V SOLID STATE SYMMETRICAL SUPERCAPACITOR USING NEEM LEAVES DERIVED ACTIVATED CARBON** *CSIR- National Physical Laboratory, Pusa Road, New Delhi, India*
12:00- 12:30	***Keynote talk*** Dr. Paula Ferreira (**I26**) **Flexible piezoelectric biomaterials for sensors** *Department of Materials and Ceramic Engineering, CICECO - Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*	Joanna Styczeń (**O13**) **The effect of the addition of synthetic zeolites on the hydration of alite** *Lublin University of Technology, Faculty of Civil Engineering and Architecture, Department of Construction, Nadbystrzycka 40, 20-618 Lublin, Poland*
12:30- 13:00	***Keynote talk*** Dr. Fábio Gabriel Nazário Figueiras (**I12**) **Thriving Narrow Band Gap Ferroelectric Oxides for Photovoltaic Applications: Bi_2ZnTiO_6 Thin Films Deposited by RF Sputtering** *IFIMUP and Departament of Physics and Astronomy, Science Faculty, Porto University; CICECO and Departament of Physics, Aveiro University*	Dr. Lidia Bandura (**O10**) **Preparation of X-type zeolite-carbon composite from fly ash and its application for petroleum products removal** *Lublin University of Technology, Faculty of Civil Engineering and Architecture, Department of Geotechnical Sciences, Nadbystrzycka 40, 20-618 Lublin, Poland*
13:00- 14:00	Lunch	

	Session: **Thin Films** CHAIR: Dr. Duncan Paul Fagg	Session: **Nanotechnology, Ceramics** CHAIR: Dr. Andrei Kovalevsky
14:00-14:30	***Keynote talk*** Aneeta Jaggernauth (**O42**) **Interfacial Integrity Enhancement of Atomic Layer Deposited Alumina on Boron Doped Diamond by Surface Plasma Functionalization** *CICECO, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*	***Keynote talk*** Dr. Indrani Coondoo (**I10**) **Phase transition studies in lead-free 50BCT-50BZT ceramics** *Department of Physics & CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal*
14:30-15:00	Session: **New Energy Materials** CHAIR: Dr. Duncan Paul Fagg Bodhoday Mukherjee (**O17**) **Electrical Transport Properties of Nickel Nanoparticles** *UGC-DAE Consortium for Scientific Research, University Campus, Khandwa Road, Indore-452001, India*	Martina Kocijan (**O19**) **The factors affecting the photocatalytic degradation of organic pollutants under visible irradiation using TiO2/rGO nanocomposites as photocatalysts** *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, Ivana Lučića 1, 10000 Zagreb, Croatia*
15:00-15:30	Session: **Hydrogen and Fuel Cell Science** CHAIR: Dr. Duncan Paul Fagg ***Keynote talk*** Prof. Dr. Yaremchenko (**I21**) **Donor- and transition metal-substituted SrTiO3: Relevant issues in the development of ceramic components for SOFC anodes** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal*	Milan Vukšić (**O20**) **Spark plasma sintering of alumina ceramics with addition of waste alumina powder** *Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia*
15:30-16:00	Coffee break	

16:00-16:30	Dr. Saloua MERAZGA (**O1**) **Properties of Mg2-x Alx Ni(x = 0, 0.1, 0.2, 0.3) alloys prepared by mechanical alloying for electrochemical hydrogen storage** *Research Center Semiconductor Technology for Energetic, Algiers, Algeria*	***Keynote talk*** Dr. Oleksandr Tkach (**I6**) **Aliovalent Doping Engineering in SrTiO3-based Electroceramics** *Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, 3810-193, Portugal*
16:30-17:00	***Keynote talk*** Dr. D. Pukazhselvan (**I28**) **Catalyzed magnesium hydride for clean energy storage applications** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*	Diogo Lopes (**O36**) **Oxide thermoelectrics prepared by laser melting: effects of processing atmosphere** *CICECO - Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
17:00-17:30	Allan J. M. Araújo (**O40**) **Proteic sol-gel synthesis of Gd-doped ceria electrolytes** *Materials Science and Engineering Postgraduate Program, UFRN, 59078-970, Natal, Brazil*	Dr. Mónica Silva (**O28**) **Cellulose acetate/Iron oxide nanocomposite films: synthesis, characterization and RB5 removal** *2C2T-Centre for Textile Science and Technology, University of Minho, Campus de Azurém, 4800-058, Guimarães, Portugal*
18:00-18:30	Francisco J. A. Loureiro (**O38**) **ZnO-modified BZY upon different B-site locations** *Centre for Mechanical Technology and Automation, Mechanical Engineering Department, University of Aveiro, Aveiro, 3810-193, Portugal*	Dr. Gabriel Constantinescu (**O37**) **Electrical performance tuning in thermoelectric Ca3Co4O9 materials by transition metals additions** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193, Aveiro, Portugal*
18:30-19:00	**Conference Closing Ceremony**	

Poster session

P1	**Synthesis and characterization of green nanocomposites based on N-carbazole** Bekkar Fadila, Bettahar Faiza, Meghabar Rachide, Hamadouche Mohammed, Leire Ruiz-Rubio *Laboratory of Polymer Chemistry, Department of Chemistry, Faculty of Science, University Oran1 Ahmed Ben bella. BP N°1524 El'Menouer, 31000 Oran, Algeria; Laboratory of Fine Chemistry, Department of Chemistry, Faculty of Science, University Oran1 Ahmed Benbella. BP N°1524 El'Menouer, 31000 Oran, Algeria; Macromolecular Chemistry Group (LABQUIMAC), Department of Physical Chemistry, Faculty of Science and Technology, University of the Basque Country, UPV/EHU, Barrio Sarriena, s/n 48940 Leioa, Spain*
P2	**The impact of β-myrcene and α - humulene on the lipid monolayers and bilayers imitating the plant pathogen bacteria membranes** Karolina Połeć, Karolina Olechowska, Katarzyna Hąc-Wydro *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Cracow, Poland*
P3	**Interaction of polychlorinated biphenyls and chlorobenzoic acids with bacterial model membrane** Aneta Wójcik, Paulina Perczyk, Marcin Broniatowski *Department of Environmental Chemistry, Faculty of Chemistry, Jagiellonian University, Kraków, Gronostajowa 2, 30-387 Kraków, Poland*
P4	**Synthesis of porous materials from fly ash** Wojciech Franus, Rafał Panek, Jarosław Madej *Lublin University of Technology, Faculty of Civil Engineering and Architecture, Department of Geotechnical Sciences, Nadbystrzycka 40, 20-618 Lublin, Poland*
P5	**The use of waste materials as ecological fillers in mix asphalt** Agnieszka Woszuk, Lidia Bandura, Wojciech Franus *Lublin University of Technology, Faculty of Civil Engineering and Architecture, Department Geotechnical Engineering, Nadbystrzycka 40, 20-618 Lublin, Poland*
P6	**Copolymerization of Maleic anhydride catalyzed by maghnite-H +** Bettahar Faiza, Bekkar Fadila, Ferahi Mohammed Issam, Leire Ruiz Rubio, José Luis Vilas *Polymer Chemistry Laboratory, Department of Chemistry, Faculty of Exact and Applied Science, University of Oran 1. Ahmed Benbella. BP No. 1542 El'Menoeur, 31000 Oran, Algeria; Department of Chemistry-Physics, Faculty of Science and Technology, University of the Basque Country (UPV / EHU), 48940 Leioa, Bizkaia, Spain;Basque Center for Materials, Applications and Nanostructures (BCMaterials), Parque Tecnologíco de Bizkaia, Ed. 500, 48160 Derio, Bizkaia, Spain*
P7	**Mesoporous material Si-MCM-41 synthesized from local kaolin DD1 as potential adsorbent for the removal of Hol Colex dye** S.Zen, Zerouali Bahya, Mekhancha Khaoula, H Mellouk, F.Z.EL Berrichi, *Laboratoire de génie civil et hydraulique, Université de 8 mai 1945, BP 401, Guelma., Algeria; Département des sciences de la matière, Université 08 Mai 1945, Guelma. Algeria; Département science de nature et de la vie, Université Mohamed Cherif Messaadia, Souk Ahras. Algeria*
P8	**The structure of non-IPR isomer 28324 (C1) of fullerene C80** Kovalenko V.I., Petrovicheva I.V., Khamatgalimov A.R. *Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, 8 Arbuzova str., 420088 Kazan, Russia; Kazan National Research Technological University, 68 K. Marx str., 420015, Kazan, Russia*
P9	**Polystyrene and Poly(ethylene glycol)-b-Poly(ε-caprolactone) Nanoparticles with Porphyrins: Structure, Size, and photooxidation Properties** Rahul K Raya, Jiří Mosinger, Pavel Kubát, Miroslav Štěpánek *Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, Hlavova 2030, 12840 Prague 2, Czech Republic; J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences, v.v.i., Dolejškova 3, 182 23 Prague 8, Czech Republic*

P10	**Encapsulation of hydrophobic bioactive substances in biodegradable polymersomes** Maria Zatorska, Urszula Kwolek, Natalia Wilkosz, Aleksandra Urych, Mariusz Kępczyński *Jagiellonian University, Faculty of Chemistry, 2 Gronostajowa St., 30-387 Cracow, Poland*
P11	**Trimethylamine oxide detection in solutions using surface-enhanced Raman spectroscopy** D.V. Novikov, S.V. Dubkov, A.I. Savickiy, D.G. Gromov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia*
P12	**Peculiarity of internal friction in nanocomposites multiwalled carbon nanotubes and polyethylene, polyvinyl chloride, expanded polystyrene** A.P. Onanko, M.P. Kulish, Y.A. Onanko, D.V. Charnyi, O.P. Dmytrenko, T.M. Pinchuk-Rugal, O.L. Pavlenko, T.O. Busko, P.P. Ilyin *Kyiv national university, Kyiv, Ukraine*
P13	**Finite element modeling of the thermal effect on the behavior of polymers under high pressure torsion process** Ahmed DRAI, Benaoumeur AOUR *Université Mustapha STAMBOULI de Mascara, Faculté des Sciences et Technologies, Département de Génie Mécanique, B.P 305, route de Mamounia, Université de Mascara, Mascara, 29000, Algérie; Laboratoire de Biomécanique Appliquée et Biomatériaux (LABAB), Ecole Nationale Polytechnique d'Oran Maurice Auden (ENPO), Oran, 31000, Algérie*
P14	**Nanoscale ferroelectricity in pseudo-cubic sol-gel derived barium titanate - bismuth ferrite ($BaTiO_3$-$BiFeO_3$) solid solutions** A.S. Abramov, A. Pakalniskis, A. Lukowiak, G. Niaura, P.Głuchowski, D.V. Karpinsky, D.O. Alikin, A. Zhaludkevich, A.L. Kholkin, R. Skaudzius, W.Strek, A. Kareiva *School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, 620000, Russia; Institute of Chemistry, Vilnius University, Naugarduko 24, Vilnius, LT-03225, Lithuania; Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okolna 2, Wroclaw, PL-50422, Poland; Institute of Chemical Physics, Faculty of Physics, Vilnius University, Sauletekio Ave. 9, Vilnius, LT-10222, Lithuania; Nanoceramics Spolka Akcyjna, Okolna 2, Wroclaw, PL-50422, Poland; Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, 220072, Belarus; Department of Physics & CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal*
P15	**In-plane polarization contribution to the vertical piezoresponse force microscopy signal mediated by the cantilever "buckling"** Lyubov Gimadeeva, Denis Alikin, Alexander Ankudinov, Andrei Kholkin *School of Natural Sciences and Mathematics, Ural Federal University, 620000, Ekaterinburg, Russia; Ioffe Institute, 26 Polytechnicheskaya, Saint Petersburg 194021, Russia; Department of Physics & CICECO - Aveiro Institute of Materials, University of Aveiro, 3810-193, Aveiro, Portugal*
P16	**Mechanical properties and thermal conductivity of epoxy composite containing aluminum-exfoliated graphite nanoplatelets hybrid powder** Kwan Han Yoon, Young Sil Lee, Jong Hun Han *Department of Chemical Engineering, Kumoh National Institute of Technology, Gumi, 730-701, Korea; School of Chemical Engineering, Chonnam National University, Gwangju 500-757, Korea*
P17	**Solid phase synthesis of calcium stearate on modified screw equipment** A.A. Momziakov, T.R. Deberdeev, A.A. Zharov *Kazan National Research Technological University, 420015, Kazan, K.Marks street, 68, Russia; Institute of Organic Chemistry, Russian Academy of Sciences, 119991, Moscow, Leninsky prospect, 47, Russia*
P18	**Improvement of active layers homogeneity for the MEA's (Membrane Electrode Assembly) of PEMFC (Proton Exchange Membrane Fuel Cell): impact of the ink quality formulation** TEAV Carine, NAYOZE-COYNEL Christine *French Alternative Energies and Atomic Energy Commission – 17 Avenue des Martyrs 38000 Grenoble, FRANCE*

P19	**Effect of adding titanium dioxide (TiO_2) on the mechanical behavior and corrosion resistance of hydroxyapatite sol–gel thin coatings on 316 L stainless steel: Biomedical application** H. KHIREDDINE, D. SIDANE, S. YALA, S. MESKI, S. ZIANI *Laboratoire de Génie de l'Environnement, Faculté de Technologie Université Bejaia, Algérie*
P20	**Photoelectrochemical properties of anodic WO_3 sensitized with $CuWO_4$** Marta Zych, Karolina Syrek, Grzegorz D. Sulka *Jagiellonian University, Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry, Gronostajowa 2, 30-387 Krakow, Poland*
P21	**Enhanced photocatalytic activity of TiO2-Ag and TiO2-Au formed on a stainless steel mesh** S. Dubkov, L. Sorokina, A. Tarasov, D. Gromov, O. Shtyka, T. Maniecki, R. Ciesielski *National Research University of Electronic Technology "MIET", 124498, Moscow, Russia; Institute of General and Ecological Chemistry Lodz University of Technology, 90-924 Lodz, Poland*
P22	**Study of the TiO2/Me structure by IR spectroscopy for use in photoactive fuel cells** S. Dubkov, L. Sorokina, A. Tarasov, D. Gromov, O. Shtyka, T. Maniecki, R. Ciesielski *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Institute of General and Ecological Chemistry Lodz University of Technology, 90-924 Lodz, Poland*
P23	**Improved performance of Silicon solar cells by ZnMgO front layer** Amel Bahfir, Messaoud Boumaour, Chaib Zoubir,Hadjira Labech *DDCS / Research Center in Semiconductors Technology for Energetic (CRTSE). 2, Bd. Frantz Fanon, B.P. 140 -7 Merveilles, , Algiers, Algeria*
P24	**Characterization of nanostructured tin oxide obtained by galvanostatic anodization** Magdalena Gurgul, Leszek Zaraska *Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian University in Kraków Gronostajowa 2, 20 – 387 Kraków, Poland*
P25	**Reactions of $BaTiO_3$ with LiH: trapping different stages of $BaTiO_3$ reduction** Hua Guo, Aleksander Jaworski, Zi Li Ma, Adam Slabon, Reji Nedumkandathil, and Ulrich Häussermann *Department of Materials and Environmental Chemistry, Stockholm University, SE-10691 Stockholm, Sweden; RWTH Aachen, 52074 Aachen, North Rhine-Westphalia, Germany*
P26	**Photoluminescence and EPR studies of single diamonds with GeV-color centers formed by ion implantation** Nikolay Lyadov, Dmitrii Zharkov, Ruslan Zaripov, Igor Yanilkin, Vladimir Nuzhdin, Valery Valeev and Rustam Khaibullin *Zavoisky Physical-Technical Institute, FRC Kazan Scientific Center of RAS, Sibirsky tract 10/7, Kazan, Russia*
P27	**Optical parameters study of amorphous germanium (α-Ge) by spectral ellipsometry** Tatyana Gavrilova, Nikolay Lyadov, Sergey Khantimerov, Nail Suleimanov, Valery Bazarov, Vladimir Shustov, Igor Yanilkin, Amir Gumarov *Zavoisky Physical-Technical Institute, FRC Kazan Scientific Center of RAS, Sibirsky tract 10/7, Kazan, Russia; Kazan Federal University, 18 Kremlyovskaya Street, Kazan, Russia*
P28	**Fluorescence properties of Nd-doped ZnO thin films obtained by the sol-gel method** Hayrullina I., Nagovitsyn I.A., Boruleva E.A., Sheshko T.F., Chudinova G.K. *Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya Str., Moscow, 117198, Russia Federation; General Physics Institute RAS, 38 Vavilov Str., Moscow, 119991, Russia Federation 3Semenov Institute of Chemical Physics RAS, 4 Kosygina Str., Building 1, Moscow, 119991, Russian Federation; National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoye shosse, Moscow, 115409, Russia Federation*
P29	**Effect on Morphology due to Dopant Elements, and Morphology-Dependent Photocatalytic Activity of ZnO Nanomaterials** Hemant Kumar Verma, H. K. Singh, K. K. Maurya *CSIR - National Physical Laboratory, New Delhi – 110012, India; Academy of Scientific and Innovative Research (AcSIR), Ghaziabad- 201002, India*

P30	**Theoretical and Experimental Properties of Ag_2SeO_3 Crystals** Ivo M. Pinatti, Ana C. M. Tello, Juan Andrés, Elson Longo, and Alexandre Z. Simões *Faculty of Engineering of Guaratinguetá, (UNESP), Guaratinguetá Brazil; CDMF, LIEC, Federal University of São Carlos (UFSCar), P.O. Box 676, São Carlos, Brazil; Department of Analytical and Physical Chemistry, University Jaume I (UJI), Castelló 12071, Spain*
P31	**Structural and optical properties of the Ag-Cu composite nanoparticles** S.V. Dubkov, A.I. Savitskiy, A.Yu. Trifonov , A.M. Tarasov, O.Shtyka, R. Ciesielski, D.G.Gromov *National Research University of Electronic Technology “MIET”, 124498 Moscow, Russia; Scientific-Manufacturing Complex “Technological Centre”, 124498 Zelenograd, Russia; F.V. Lukin State Research Institute of Physics Problems, 124498 Zelenograd, Russia; Lodz University of Technology, 90-924, Lodz, Poland*
P32	**The influence of selected cationic derivatives of phosphatidylcholines on the properties of model mammalian membranes** Marzena Mach, Magdalena Kowalska, Paweł Wydro *Department of Physical Chemistry and Electrochemistry, Jagiellonian University, Gronostajowa 2 30-387 Krakow, Poland*
P33	**The study of the impact of lipid structure on their interactions with 2-hydroxyoleic acid** Łukasz Płachta, Karolina Olechowska, Magdalena Kowalska, Marzena Mach and Paweł Wydro *Department of Physical Chemistry and Electrochemistry, Jagiellonian University, Gronostajowa 2 30-387 Krakow, Poland*
P34	**The influence of bisphenols on the properties of model human erythrocyte membranes** Karolina Olechowska, Beata Wyżga, Karolina Połeć, Katarzyna Hąc-Wydro *Department of Environmental Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387, Kraków, Poland*
P35	**Optical and Structural Properties of $Cu_2Zn_{1-x}Cd_xSnS_4$ Thin Films Obtained by Ultrasonic Spray Pyrolysis** O. Mohammed Cherif, A. Meftah, N. Attaf *Département de physique , Faculté des sciences, Université 20 Août 1955-Skikda, Algérie; Département de physique, Faculté des Sciences exactes, Université de Constantine Algeria, Algeria*
P36	**Thermal stabilization of geometric parameters at 100°C of a silver nanoparticles array obtained by vacuum-thermal evaporation on a unheated substrate** D.G. Gromov, S.V. Dubkov, G.S. Eritsyan, A.I. Savitskiy, V.A. Bykov, Yu.A. Bobrov *National Research University of Electronic Technology (MIET), Mocsow, Russia; SMC Technological Center, Moscow, Russia; LLC “NT-MDT”, Moscow, Russia*
P37	**The influence of the PEG-ylation degree of 1,2-disteroil-sn-glycero-3-phosphoethanolamine on the molecular organization of model lipid membranes** Magdalena Kowalska, Marzena Mach, Łukasz Płachta, Paweł Wydro *Department of Physical Chemistry and Electrochemistry, Jagiellonian University, Gronostajowa 2, Krakow, 30-387, Poland*
P38	**An Investigation on 100 MeV Ni7+ Swift Heavy ion Irradiation effect on the Ferroelectric Triglycine Sulphate <011> Oriented Single crystal** V.C. Bharath Sabarish, G.Ramesh Kumar, A. Durairajan, S.Gokulraj *Department 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*
P39	**Influence of tungsten RDE rotation on the morphology of anodic WOx formed in NH4NO3-based electrolyte** V.A. Benu, Y. V. Nazarkina, E.M. Eganova *National Research University of Electronic Technology “MIET”, 124498 Moscow, Russia; Establishment of the Russian Academy of Sciences, Institute of Nanotechnology Microelectronics INME of RAS, Leninskiy Prospekt 32A, Moscow, 119991, Russian Federation*

P40	**Influence of thermal treatment parameters on functional properties of multi-walled TiO2 NTs** A. Dronov, T. Savchuk, I. Gavrilin, M. Kamaleev, D. Dronova, T. Maniecki, S. Gavrilov and D. Gromov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Lodz University of Technology, Lodz, Poland*
P41	**Electrochemical properties of electrodes based on anodic TiO2 nanotubular layers for Al-ion batteries** D.A. Dronova, A.S. Gavrilov, A.A. Dronov *National Research University of Electronic Technology "MIET", 124498 Moscow, Russia*
P42	**Effect of adsorption of epoxide and hydroxyl group on a monolayer graphene sheet: A DFT investigation** Budhendra Singh, Igor Bdikin, V. Bystrov *Department of Physics, Central University of South Bihar, SH-7, Gaya-Panchanpur Road, P.O. Fatehpur, P.S. Tekari, Gaya – 824236, India; TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, 3810-193, Aveiro, Portugal; Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia*

Plenary Lectures

Computer modeling and calculations of physical properties of self-assembled nanostructures based on various amino acids (review)

Vladimir Bystrov *

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The review is devoted to the analysis of molecular models of various nanostructures and peptide nanotubes (PNT) based on a number of amino acids (AA), the computer methods used here and the results obtained in comparison with known experimental data. Self-assembly of complex AA molecular structures is one of the most important phenomena both in living nature and in artificial biomimetics. This is important for our understanding of wildlife, as well as for numerous practical applications (in particular for targeted drug delivery).

A necessary research approach here is computer molecular modeling of the processes of self-organization of molecular systems at the different levels and by different methods. All AA have their own dipole moments, which interact with each other and self-organize into more complex molecular and crystalline structures, such as PNT. Many of these structures have piezoelectric and ferroelectric properties.

Self-assembly of such PNT occurs in aqueous media rather quickly and under certain conditions that affect the rate of their growth, the shape of self-organizing structures.

In many cases, water molecules also appear in the internal hydrophilic cavity of such PNT. They affect the physical properties of PNT and largely determine their changes. However, the experimental detection of water molecules by X-ray diffraction methods is very difficult. It is computer simulation methods that play an important role in the identifying these water molecules and establishing their structural and physical properties, the effect on the properties of PNT as a whole.

Computer molecular modeling allows one to calculate, investigate and predict the basic physical properties of these nanostructures based on various AA. As it is known not only diphenylalnine (FF) PNT, having aromatic (benzene) rings, exhibit piezo / ferroelectric properties. Branched chain AA (BCAA) are known (isoleucine (I), leucine (L) and valine (V)) also exhibit piezo / ferroelectric properties.

Piezoelectric Nanoparticles Based Flexible Nanogenerators

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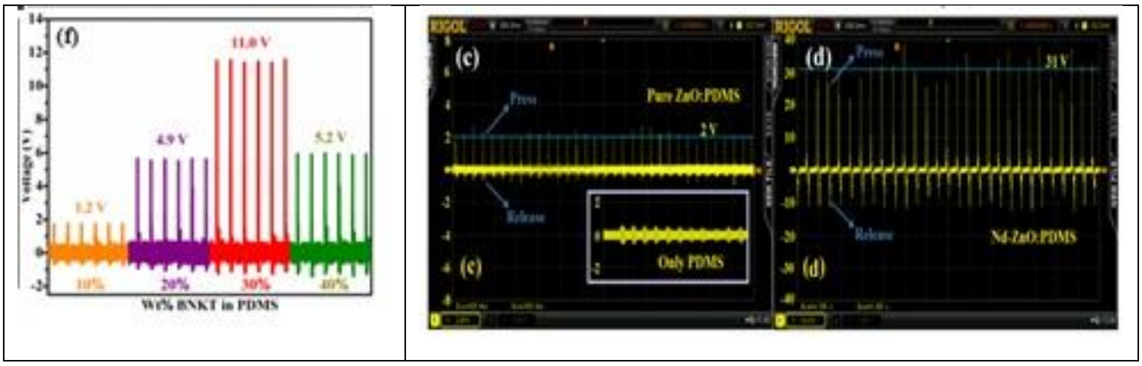
High performance piezoelectric nanoparticle based flexible NanoGenerators (NGs) are future alternate energy source to harvest energy directly from local environment like finger tapping, walking, breathing, etc [1]. In the present talk, the basic of nanoparticle performance and the recent achievements on the application of piezoelectric nanoparticles for green energy will be presented.

ZnO is a versatile material which exhibits interesting ferroelectric, piezoelectric, optical, etc. properties when doped with various rare earth elements [2,3]. As a result of doping, enhanced piezoelectrical charge coefficient were achieved in different ZnO structure, synthesized by wet chemical route, showing different morphology for improved performance of piezoelectrical devices. Similarly, some other high performance piezoelectrical nano/microsystems, including lead based perovskite BNKT and (KNN-BNZ) were synthesized by high temperature solid state reaction followed by ball milling [4,5]. These nanoparticles were characterized for structural (XRD), morphological (FESEM/HRTEM), dielectric, ferroelectric, piezoelectric and optical (PL, Raman, UV-Vis), etc properties.

The synthesized piezoelectric nanocrystals were used, both as direct nanostructure as well as in the form of thick flexible composite tapes. For this, thick tape of piezoelectricnano-crystals / PDMS on ITO/PET substrate were fabricated by spin coating. The generation of electrical energy by simple finger tapping and using force simulater was studied. Applied force and its frequency were varied in the range of 0.3 N- 20N and 5 Hz – 100 Hz, respectively. High voltage output in the range of 0.5 – 50 V were obtained. It has been demonstrated that the synthesized piezoelectric nanocrystals can be used for energy harvesting.



1. Y-doped ZnO nanosheets: Gigantic piezoelectric response for an ultrasensitive flexible piezoelectric nanogenerator, Ceramics International 44 (2018) 8582
2. A review on piezo-/ferro-electric properties of morphologically diverse ZnO nanostructures, JALCOM 816 (2020) 152491
3. Tb-doped ZnO:PDMS based flexible nanogenerator with enhanced piezoelectric output performance by optimizing nanofiller concentration, Ceramics International (2020) In Press
4. Lead-free 0.95(K0.6Na0.4)NbO3-0.05(Bi0.5Na0.5)ZrO3 ceramic for high temperature dielectric, ferroelectric and piezoelectric applications, JALCOM 818 (2020) 152874
5. Flexible lead-free piezo-/ferroelectric Bi0.5(Na0.6K0.4)0.5TiO3 ceramic incorporated PDMS polymer composites for energy harvesting application, Journal of Materials Science: Materials in Electronics, 30 (2019) 6157

Spatio-temporal dynamics of active catalysts observed by multi-scale in-situ electron microscopy

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Modern analytical transmission electron microscopes are capable of delivering picometer resolved information about the geometric arrangement of atoms. It is possible to simultaneously obtain quantitative information about the elemental composition of a material and even to measure the local electronic structure or electric and magnetic fields. One of the side-effects of using strongly interacting electrons for the imaging process is the requirement of a good vacuum near the sample and throughout the optical system. Obtaining detailed information about the state of an isolated material in vacuum is not sufficient if we are interested in processes such as material growth- and decomposition, corrosion or (electro)catalysis. With the availability of MEMS- (micro electro mechanic systems) technology based TEM holders for *in situ* experiments, it is now possible to study the response of a material to a physical or chemical stimuli and study gas-phase, temperature and electrochemically induced processes. Since atomic motions can be fast and the temporal resolution of conventional microscopes is limited and furthermore, processes are often related to collective dynamics of many atomic species, a combination of high-resolution imaging with context embedded observation at lower magnification is required.

In my presentation I will show how the combination of *in situ* scanning and transmission electron microscopy enables a multi-scale approach for the study of functional materials in their relevant state. Examples range from CVD growth of 2D materials [1] to redox dynamics [2] and catalysed surface reactions [3]. It will be shown how *in situ* microscopy reveals the beauty of complex dynamics in systems that are operated far from thermodynamic equilibrium.

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Ion beam modification of magnetic anisotropy, interlayer coupling and tunnel magnetoresistance in magnetic tunnel junctions

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Magnetic properties of materials are dependent on the structure, from the coupling to the lattice to the emergence of effective anisotropies caused by the microstructure-related spatial-dependent magnetization. Interfacial magnetic phenomena and interlayer interactions may be modified by ion irradiation [1-3]. That provides a route for the control of magnetism in multilayer stacks, namely in magnetic tunnel junctions (MTJ) [4]. Before applications can be envisaged, however, it is necessary to understand the full extent of effects produced by the irradiation on the interface-controlled parameters of MTJ stacks. Thus, we irradiated an MTJ with 400 keV Ar+ ions at several fluences. The magnetic part of the stack was IrMn/PL/Ru/RL/MgO/FL/Ta/Ru, where PL, RL and FL are pinned, reference and free layers made of CoFe. Ferromagnetic resonance was used to measure the effective anisotropy field of the FL, comprising interfacial perpendicular anisotropy (PMA) and shape anisotropy. All magnetic layers were in-plane magnetized. The anisotropy keeping that in-plane magnetization decreased with the ion fluence, resulting from the stronger decrease of magnetization, due to induced intermixing at the FL/Ta interface, than of PMA at the MgO/FL interface. The tunnel magnetoresistance (TMR) decreased following a decrease in the resistance of the antiparallel state, due to the creation of defects within the MgO barrier, acting as spin-independent tunneling channels shunting the spin-dependent one. At the higher fluence range the RL became decoupled from the PL and the TMR vanished. We show there is a window of operation for tuning the magnetic anisotropy using ion irradiation, while retaining interlayer coupling and TMR required for MTJ applications.

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Graphene: From fundamental research to technological applications

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Although pristine graphene is one of the most relevant materials of the past decade, several important shortcomings must be overcome before it can step from fundamental physics to applied technology, while preserving its amazing properties. Today, we have developed strategies to grow high quality graphene on top of a metal surface [1], but the surface-graphene interaction quenches them. Several strategies have been implemented to decouple graphene form the surface to avoid transferring of the layer, a process that degrades the properties [2-4].

Another important aspect that needs to be solved it is related to its extreme chemical inertness and the absence of an electronic band-gap, which impose limitations to its use as an active element in electronic devices and hybrid structures. Thus, technologically useful and robust graphene-based interfaces for nano-bio-hybrid devices require highly selective, stable and covalently bonded functionalities on the graphene surface. In this talk, we describe a relatively straightforward route to the covalent chemical functionalization of graphene sheets, with any amino containing molecules, as anchoring group [5]. We employ a recently reported and patented strategy [5,6] for the selective functionalization of graphene through the controlled formation of atomic vacancies. The result is a controlled decoration of the graphene surface with active thiol moieties, which can subsequently be directly used to bind diverse nanoarchitectures to graphene. We have used this strategy to covalently couple two systems of broad interest: gold nanoparticles (Au-NPs) [6] and thiol-modified nucleic acid aptamers.

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Site-controlled Nucleation in Ordered Array of Epitaxial SiGe Quantum Dots: Growth, Properties and Application

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SiGe-based quantum dots (QDs) heterostructures are very attractive for device application due to its compatibility with standard developed Si technology. To be implemented in next generation CMOS-compatible with nano-electronic and optoelectronic devices they can be formed in regular and uniform arrays with controlled size, shape, chemical composition, and the properties of their surrounding like choice of matrix material.

For realistic integration of QDs into Si-technology devices, the QDs have to be site-controlled to ensure their large scale addressability. Besides, ordered array of QDs provide several more benefits as compared to their randomly nucleated counterparts: a more homogeneous chemical composition and energy spectrum.

In this report, we will focus on self-assembled, group-IV, Ge-on-Si epitaxial QDs, formed during with dislocation-free growth [1].

The modelling and experimental research the effects of elastic strain and pit-patterned surface prepared with electron beam lithography or ion-beam action on nucleation and epitaxial growth of ordered groups SiGe quantum dots are shown.

To demonstrate device application for nanophotonic the collective effects on enhancement of infrared light absorption/emission in silicon based nanostructures have been studied. The integration of nanostructures with metallic metasurfaces as a metallic film perforated with a subwavelength hole array are employed as plasmonic couplers to convert the incident electro-magnetic radiation into surface plasmonic waves. The results demonstrate that plasmonic structure on the top of quantum dot nanostructures are very efficient approach for light absorption and light emission enhancement in silicon based nanostructures.

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Acknowledgement

The work was funded by Russian Scientific Foundation (grant 19-12-00070).

Invited Speakers

I1. Self-assembled diphenylalanine microtubes: structure, characterization and application

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The diphenylalanine (H-Phe-Phe-OH, FF) is one of the self-assembling peptides which have recently become a focus of intensive research in the field of nanomaterials because they can spontaneously form fascinating discrete and well-ordered structures: nano- and microtubes, nanospheres, nanofibrils, and hydrogels. FF peptide nanotubes (PNTs) possess unique biological and physical properties such as biocompatibility, high rigidity [1], notable thermal stability, interesting electronic, nonlinear optical and photoluminescent properties, as well as exceptional piezoelectric effect [2] and pyroelectricity. Thus FF PNTs represent a promising functional material for various nanoelectronic applications (piezoelectric sensors, actuators, micromechanical systems, resonance biosensors etc)

In this work, we report the results of our recent studies on the growth and characterization of FF PTs by different methods. Low temperature phase transitions were rigorously studied by dielectric spectroscopy. Several anomalies were found in the temperature range 100-350 K accompanied by the strong dielectric relaxation. Unusual behavior of the dielectric relaxation time observed in this work was attested to the relaxation of water molecules existing in the FF PTs nanochannels. At low temperature two groups of water molecules coexist near the hydrophilic carboxyl groups and in the core of nanochannels having completely different dynamics leading to structural changes. A crucial role of nanoconfined water in emerging physical properties of FF peptide tubes will be discussed in this work.

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Acknowledgment

This work was supported by FCT through the project “BioPiezo”- PTDC/CTM–CTM/31679/2017

I2. Magnetic properties of (1-x)BiFeO$_3$ – xBaTiO$_3$ ceramics across the phase boundary

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Materials based on bismuth ferrite attract great attention of the scientific community due to wide variety of structural and magnetic phase transitions [1-2]. Solid solutions based on bismuth ferrite have certain disadvantages - low residual magnetization, small magnitude of magnetoelectric interaction, etc., which significantly limit the scope of their possible applications. Substitution of the perovskite lattice in A- and B- positions using alkaline earth ions and transition metals can eliminate these disadvantages and allow to control the crystal structure of the compounds and their magnetic properties. A correlation between the crystal structure and magnetic properties of the co-doped compounds have been studied for solid solutions (1-x)BiFeO$_3$ – xBaTiO$_3$ using X-ray diffraction and magnetometry techniques.

The structure of the compounds with x < 0.3 is described by single phase state with rhombohedral symmetry of the unit cell, the dopant increase leads to a reduction of structural distortion. Magnetization measurements performed for the compounds with x < 0.3 have revealed dominant antiferromagnetic structure with small remanent magnetization (~0.015 emu/g) caused by non-collinear alignment of the magnetic moments. Increase in the dopant concentration cancels the remanent magnetization. The evolution of magnetization is caused by a change in symmetry of the crystal structure from the rhombohedral to the (pseudo)cubic phase.

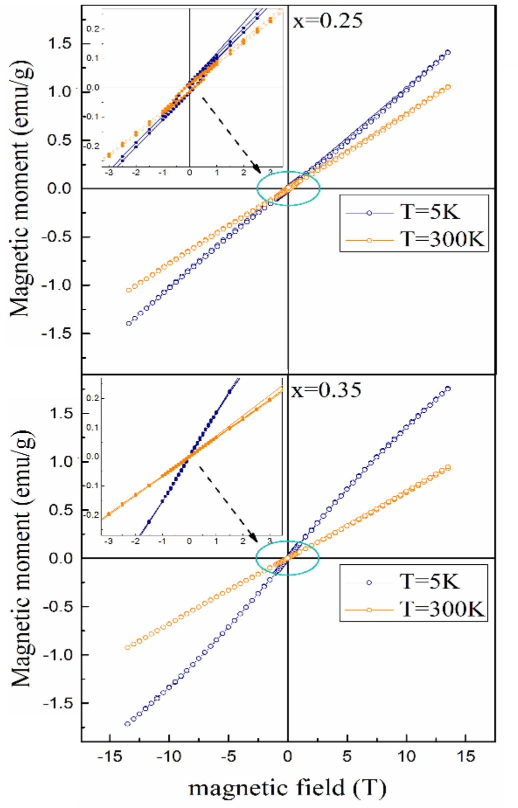

Fig. 1. Field dependences of magnetization obtained for (1-x)BiFeO$_3$ – xBaTiO$_3$ compounds with x = 0.25 and 0.35 at temperatures T = 5 K and 300 K. The insets show magnified parts of the magnetization curves near the origin.

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I3. Structure and magnetic properties of Sm doped BiFeO$_3$ ceramics across the rhombohedral-orthorhombic phase transition

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The phase diagrams attributed to multiferroic compounds based on BiFeO$_3$ suggest strong correlation between the crystal structure and physical properties [1, 2]. The correlation is mainly governed by electronic configuration and ionic radii of the dopant ions while structural morphology of the compounds can also affect the “structure-property” concept. In the present study the correlation is investigated for compounds Bi$_{1-x}$Sm$_x$FeO$_3$ prepared by sol-gel and solid state reaction methods.

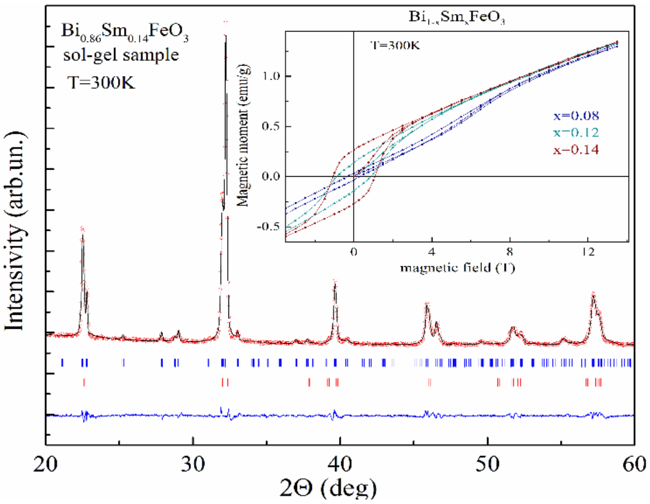

Figure 1. X-ray diffraction pattern of the compound Bi$_{0.86}$Sm$_{0.14}$FeO$_3$ prepared by sol-gel method. The insert shows M(H) dependences of the sol-gel compounds with x = 0.08 - 0.20 measured at 300K.

The crystal structure of the compounds with $x \le 0.12$ is polar rhombohedral (s.g. R3c) regardless the synthesis method. Increase in the dopant content leads to the structural transition to the anti-polar orthorhombic structure (s.g. Pbam) via narrow two phase region (Fig. 1). Magnetic properties of the solid state compounds are characterized by distinct modification of the magnetic structure occurred at the structural phase transition [3]. The isothermal magnetization dependences obtained for the compounds prepared by sol-gel method show gradual increase in the remnant magnetization and coercivity with dopant content without any correlation with the structural transition (Fig. 1, inset). The difference in the magnetic properties is most probably determined by nanoscale crystallines of the sol-gel compounds which causes a disruption of the modulated magnetic structure and release of spontaneous magnetization already in the rhombohsdral phase.

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I4. Nanoscale inhomogeneity in oxide single crystals: NiO and $Ni_{1-x}Li_xO$ case

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Metal-oxide (MO) compounds are a wide class of materials, the interest in which is due to both the great potential for technical use and the variety of physical properties of interest from the point of view of fundamental research. Nickel oxide (both undoped and doped by Li) has a special interest because of physical properties. It is known that the properties of most metal-oxide compounds are extremely sensitive to the presence of defects and inhomogeneities of various types in the investigated samples. Therefore, study of real structure of high quality single crystals and thin films of MO compounds is an important task of material science.

The (100) surface of NiO and Li doped NiO single crystals grown by floating zone melting were studied after ion bombardment and annealing in UHV by photoemission spectroscopy, XRD , LEED, AFM and STM/STS. 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. 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_y oxides are coupled coherently through common structural elements.

This work was supported by RFBR Grant 19-29-03021

I5. The effect of synthesis temperature on the microstructure and electrophysical properties of multifunctional BST thin films

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Thin ferroelectric layers embedded into heterostructures are of interest both to fundamental research and to electronic applications. Barium titanate doped with strontium having perovskite structure is a common ferroelectric material with a high dielectric constant. It is an attractive material for applications such as multilayer capacitor, pyroelectric detectors, dynamic random access memory device, non-volatile memories, integrated circuit technology etc. Properties of film structures strongly depend on their fabrication, electrode materials and substrate. Polarization ordering and switching dynamics are among the most important issues in the physics of ferroelectrics. They should be addressed before considering any practical applications. In this work, we have systematically studied electrical, dielectric, ferro- and piezoelectric properties of $Ba_{0.8}Sr_{0.2}TiO_3$ (BST 80/20) films in order to understand its functional properties for future flash memory applications. Ferroelectric BST 80/20 films with thickness in the range 150-550 nm were prepared by the high-frequency reactive sputtering on different substrate materials (SiO_x/Si and Pt/TiO_2/SiO_2/Si). For measurements of electrical and dielectric characteristics on the automated experimental setup, dot-shaped Ni top electrodes were deposited on the surface of BST films using a shadow mask by the vacuum evaporation. The surface morphology, local piezoelectric response and surface potential images of BST 80/20 films were measured by the scanning probe microscopy MFP-3D SA (Asylum Research, USA) in the Piezoresponse and Kelvin Probe modes. The obtained results point to the fact that the BST ferroelectric thin films are promising materials for using as memory elements.

This work was carried out as part of a state assignment and was partially supported by the Russian Foundation for Basic Research (projects nos. 18-29-11029, 19-07-00271 and 19-29-03042).

I6. Aliovalent Doping Engineering in $SrTiO_3$-based Electroceramics

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Development of giant-permittivity and high-tunability dielectric materials has attracted great interest because of growing demand for smaller and faster energy-storage and electronic devices [1-3]. Materials such as $CaCu_3Ti_4O_{12}$, displaying the giant dielectric permittivity due to extrinsic Maxwell-Wagner interfacial polarization effect, have previously been reported. Ferroelectric materials possessing intrinsic ionic polarization due to a phase transition to the polar state have also been indicated to possess high dielectric permittivity. Here, a class of the giant-permittivity materials based on $SrTiO_3$ ceramics doped with about 1% of trivalent ions like yttrium, dysprosium and gadolinium as well as their processing concept, which yields the dielectric permittivity up to ~209 000 at 10 kHz, is reported [1,4-6]. The giant permittivity is explained by a coupling of the polar clusters relaxation mode with the donor substitution induced electrons at low temperatures and by the Maxwell-Wagner relaxation around room temperature. Besides the fundamental understanding, this discovery opens a new development window for high-frequency and low-temperature electronic and energy-storage applications.

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I7. Graphoepitaxial 3DGE growth of multilayer thin film heterostructures

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Multilayer heterostructures of metal oxides were fabricated on $NdGaO_3$ (NGO) tilted-axes substrates (TAS) with pulsed laser deposition, orientational features of the layers were studied with XRD techniques.

A deviation of the film surface from the standard crystallographic plane of epitaxial growth (the (110) plane of NGO in our case) often results in graphoepitaxial matching between the film and the substrate (the 3DGE growth mechanism) instead of the standard epitaxial parallelism between crystallographic planes of film and substrate. We studied graphoepitaxial relations in multilayer heterostructures and found three main variants.

The trivial case demonstrates graphoepitaxial matching on all interfaces of the heterostructure. The geometrical nature of the 3DGE mechanism results in an inheritance of orientational relations through the whole structure, and the top layer shows the same orientation as if it was grown directly on TAS, with no influence of the intermediate layers. This variant was most often observed with relaxation of a strained film: the orientation of the film changes with thickness according to the relaxing out-of-plane lattice constant.

A more complicated structure is observed when the orientation of intermediate layer is influenced by another, non-3DGE, tilting mechanism. In this case the surface of each bottom layer acts as an independent TAS for growth of the top layer. The orientation of the top layer was determined by the 3DGE growth mechanism, but exact orientation differs from the purely-3DGE case.

The third variant is realized when an interlayer is formed between the layers of the heterostructure, usually as a result of chemical interaction between the deposited material and the surface of the bottom layer. This interlayer shows standard epitaxial relations either with the bottom layer, or with top layer of the heterostructure, providing completely different orientation of the top layers of the multilayer grown with the 3DGE mechanism.

The work was supported by Program of Ministry of Science and Higher Education of Russian Federation. I.K.B. wishes to acknowledge FCT for its financial support (grant IF/00582/2015).

I8. Structural, Optical and Mechanical property of pure and Sulphur doped Gallium Selenide: A first Principle study

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Gallium Selenide □□□GaSe), a layered semiconductor bulk crystal of III-VI compound, has attracted much attention due to its non-linear optical (NLO) properties along with a high damage threshold and a high transparency for near infrared wavelength (0.65–20 µm)[1-3]. Due to this, it is extensively used in infrared frequency conversion, non-linear optical devices and photodetectors[4]. Among the various doping elements Sulphur (S) doped GaSe has an interesting feature due to isovalent, having similar size and forming isostructural binary compounds of S and Se atoms. In the present paper, the structural, electrical and optical properties of $GaSe_{1-x}S_x$ alloys (x= 0, 0.25, 0.5, 0.75, 1) have been studied with in DFT (density functional theory) framework using Quantum Espresso (QE) package [5]. For testing the exchange and correlation effect, separate calculation with local density approximation (LDA) [6] as well as generalized gradient approximation (GGA) [7] were carried out for the exchange-correlation functional. Electron-ion interaction was treated with pseudopotential method. An optimized, highly accurate non conversing pseudopotential files with valence electron configuration $3d^{10}4s^{2}4p^{1}$, $4s^{2}\,4p^{4}$, and $3s^{2}3p^{4}$, for Ga, Se and S atoms, respectively were directly used from pseudo-dojo library for all calculations [8]. After testing for convergence of various parameters, the kinetic energy cut-off was set to 90 Ry while the charge density cut-off was set to 360 Ry. The integration over the brillouin zone (BZ) was performed employing 10 x 10 x 2 Monkhorst–Pack (MP) k-points mesh. Checking with a more condensed k-points sampling and a larger kinetic energy cutoff in the present case did not resulted in any significant change in the ground state energy. The difference in the energy was found to be less than 0.01 meV. The atoms in the structure were fully relaxed to till all forces became smaller than $10^{-3}\ eV/Å$. The energy convergence parameter was set to $10^{-8}\ eV$. For substitution, specific number of Selenium was replaced by Sulphur in □-GaSe phase and by Selenium in □-GaS phase. For accurate comparison of results MP grid for pure and substituted structure was kept constant. The density functional perturbation theory (DFPT) as implemented in the phonon code with QE [7, 9] was used to calculate phonon frequencies at G q-points for evaluated the Raman and IR spectrum. For all other property calculation thermo_pw package integrated with QE- version 6.3 [10] was used. The results were analyzed and discussed in detail.

Conclusion

The effect of Sulphur substitution on GaSe was evaluated using DFT calculation. The calculated lattice parameters show a good approximation along xy plane using LDA and GGA functional, however along z axis these functional seems to overestimate the parameter due to Vander wall interaction between layers. A comparatively good approximation was achieved using local vander-wall correction (DFT-D3) with GGA functional. The various results were discussed and effect of vander-wall correction on various physical properties were compared and explained.

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I9. Manganese substitution effect on the structural, optical, magnetic and magnetocaloric properties of $HoCrO_3$ orthochromite

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The effect of moderate Mn substitution (at Cr-site) on the physical properties (including structural, optical and magnetic) of $HoCr_{1-x}Mn_xO_3$ (x = 0, 0.15) has been thoroughly investigated. A detailed structural analysis of the samples provided a way to correlate the optical and magnetic properties with the change in Cr-site ionic radii, tilt angles and distortion in Cr/MnO_6 octahedra. Further, variation in the phonon modes was associated with structural distortion owing to Mn substitution in $HoCrO_3$ (HCO) compound. The octahedral distortion variation was found to be closely related with Urbach energy values measured from diffuse reflectance spectroscopy. The optical band gap reduced from 3.12 eV to 2.04 eV after Mn substitution. The overall structural distortion with Mn substitution resulted in the decrease of antiferromagnetic transition temperature of the pristine compound. The strong magnetic entropy change was observed at low temperatures in pure HCO compound and its value was found to enhance with Mn substitution. Therefore, our work provides a convenient method to tune the multifunctional properties of HCO compound which have practical applications such as photocatalyst and low-temperature magnetic refrigerant.

I10. Phase transition studies in lead-free 50BCT-50BZT ceramics

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$(Ba_{0.85}Ca_{0.15})(Zr_{0.10}Ti_{0.90})O_3$ or 50BCT-50BZT is one of the most popular and technologically important lead-free piezoelectric composition, which has been extensively studied in recent past. It exhibits outstanding electromechanical properties such as $d_{33} >$ 500 pC/N and $d^*_{33} >$ 1000 pm/V at 0.5 kV/mm [1]. The sequence of phase transitions in this material has remained controversial from the beginning owing to contradictory results obtained by various research groups. Therefore, through this study we have made a sincere effort to resolve the phase transition related issues in this compound. Bulk ceramics of the composition 50BCT-50BZT were synthesized using two techniques: solid state reaction and sol-gel method. An exhaustive analysis of the results obtained in a broad temperature range using various experimental techniques: x-ray diffraction, Raman scattering, dielectric and Piezoresponse Force Microscopy (domain configuration studies), provided clear evidence of phase transition sequence similar to that in the parent barium titanate and another “R3c → R3m” at lower temperature.

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I11. Strontium titanate and zinc-oxide-based materials for high-temperature thermoelectric harvesting

Andrei V. Kovalevsky [1, *], Kiryl V. Zakharchuk [1], Nuno M. Ferreira [2], Wenjie Xie [3], Sonia G. Patrício [1], Blanca I. Arias-Serrano[1], Sergey M. Mikhalev [4], Diogo Lopes [1], Gabriel Constantinescu [1], Sergii A. Sergiienko [1], Florinda M. Costa [2], Jorge R. Frade [1], Anke Weidenkaff [3]

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Broad societal needs have focused increased attention to providing a sustainable energy supply to the population, based on technologies with minimal environmental impact and reduced fossil fuels usage. One solution is to improve energy conversion efficiency in key consuming sectors. Since most of the energy (60-70%) used worldwide is discharged as waste heat, ”green” thermoelectric (TE) conversion has received considerable attention due to its intrinsic simplicity, employing no moving parts, silent operation, excellent scalability and reliability, and self-sufficiency to enable mobile or remote applications. In some energy-conversion scenarios, the cost and thermal stability requirements may dominate over efficiency issues, making abundant, high-temperature-stable and low-toxic oxides an interesting alternative TE material. This talk will feature some oxide-specific approaches towards tuning the thermoelectric performance in strontium titanate and zinc-oxide-based materials, including defects engineering and in-situ induced nanostructuring.

I12. Thriving Narrow Band Gap Ferroelectric Oxides for Photovoltaic Applications: Bi_2ZnTiO_6 Thin Films Deposited by RF Sputtering

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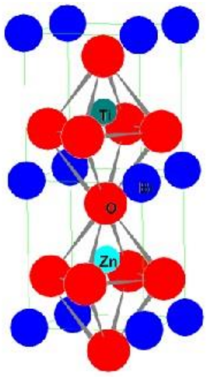
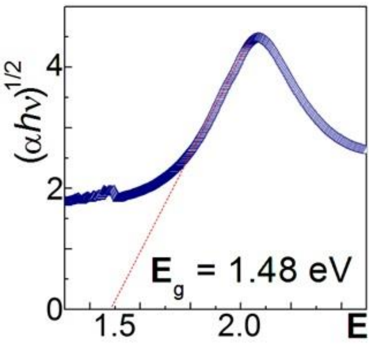
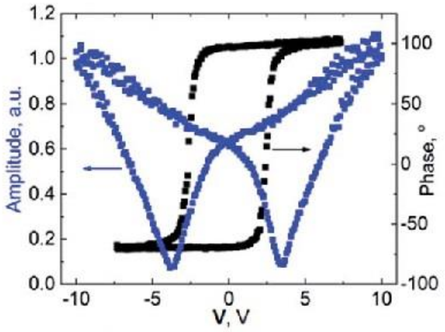
The formation of a ferroelectric Bi_2ZnTiO_6 (BZT) perovskite-like phase in the thin film form is demonstrated to be viable onto Pt/Si-based substrates at 550 ºC using the rf-sputtering method. This “lead-free” BZT polycrystalline phase has a noncentrosymmetric P4mm tetragonal structure, exhibiting a noteworthy piezoelectric response and an optical gap of 1.48 eV in agreement with the theoretical calculations. Further research and development of BZT thin films can be regarded as a thriving material for innovative generation of optoelectronic and photovoltaic devices where the intrinsic polarization field can replace the function of p-n junctions in semiconductors [1].







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I13. Localized corrosion at zinc-galvanized surface and corrosion prevention strategies

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The society and global regulations put demands on the automotive industry to make vehicles safer, more sustainable and affordable. Following such goals structural materials in vehicles are replaced by different metallic materials and composited for improving the overall performance. Galvanic corrosion of metals is a significant problem where multilaterals are intensively used. More knowledge is needed concerning the corrosion degradation and interface stability and corrosion susceptibility of metallic materials and their combinations in different corrosive environments. Corrosion susceptibility at the cut-edge is one of examples where there is a high risk of losing mechanical integrity of structural parts due to corrosion. Therefore the knowledge of localized corrosion activity of galvanized steel, which is a common material in automotive industry, is very important.

The main objective of the present work is analysis of local failure mechanisms of different galvanized layers. Particular objectives involve studies of local corrosion initiation at the cut-edge of adhesively bonded galvanized steel and corrosion susceptibility of different metallic phases found in zinc galvanized layers. The second objective was to explore various protective coatings for zinc galvanized layer. This has been done by applying inorganic coatings Layered double hydroxides (LDH) and oxidic layers which are aimed at improving mechanical and active corrosion protective properties of the underlying metal. Main methods of analysis were in situ atomic force microscopy (AFM), EC-AFM and supportive methods such as electron microscopy (SEM), energy dispersive spectroscopy (EDS), X-ray diffraction.

It has been shown that various localized corrosion events occur at zinc galvanized layers. Local corrosion spots were identified in situ and their location depends on phase composition of the galvanizing layer and applied electrochemical conditions. Utilizing inorganic coatings such as LDH with or without oxide layers may improve corrosion protection of zing based materials and decrease galvanic corrosion susceptibility.

I14. Negative dielectric permittivity material based on La and Pr doped $EuMnO_3$ perovskite system

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Perovskite multi-ferroics with a negative value of the dielectric constant are useful materials because of their applicability in electronic devices. In this work, the Lanthanum (La) and Praseodymium (Pr) doped in $EuMnO_3$ ceramics with the general formula $K_{1-x}Eu_xMnO_3$ (where x = 0.10, and K = La and Pr) has been synthesized via Solid-state method. The weighed raw materials were mixed according to the solid-state reaction method for 7h in the presence of acetone medium. Then the powder was dried at 120^0C and calcined at 1000˚C for 4 h. These ceramics pellets are obtained by the sintering process at 1200˚C for 4 h in a closed alumina crucible in the presence of air. Here we will present the result of the structural and electrical (dielectric/modulus) studies on perovskite manganite $K_{1-x}Eu_xMnO_3$ synthesized by solid-state reaction method. Powder X-ray diffraction pattern and Rietveld analysis revealed that all the samples are crystalline in the space group of *R3-c* with *the* rhombohedral crystal structure. The tolerance factor decreases with increasing the X content in the composition, which confirms the calculated structure from Rietveld analysis. The crystallite size of $K_{1-x}Eu_xMnO_3$ samples found in the range of 50 nm-70 nm. The complex impedance plot exhibited one semi-circle at higher temperatures, and the centers of the semicircles lie below the real axis, which indicates that the material is the non-Debye type. The single impedance semicircle confirmed the bulk grain effect in samples. Bulk resistance decreased with the increase of temperature, which confirmed the negative temperature coefficient of resistance behavior (NTCR). Real dielectric permittivity increases with increases in temperature and decreases with increases in frequency.

I15. Modeling electrons in solids, surfaces and nanostructures (with an introduction to density functional methods)

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Density functional theory (DFT) has been a trustful workhorse for predicting and reproducing a wide range of experimental observables. It gives us access to a quantum-mechanical picture of an electronic gas under the influence of thousands of nuclei. Density functional theory and spectroscopy techniques are, in many aspects, inseparable partners in a modern laboratory, and played decisive roles in the identification and understanding of a vast amount of problems on solid-state physics, surface science and nanotechnology. In this talk I will explain the workflow of DFT modeling, why it has been so successful, and along the way, a few successful stories will be told, including how we found the workings of major carrier-life-time-limiting traps in semiconductors, the flipping-dynamics of reconstructions on semiconductor surfaces, the recent identification of the defect responsible for the light-induced degradation of the power conversion efficiency of Si solar cells, or the mechanism for electron-transfer within a network of silicon nanocrystals.

I16. Alternative strategies for biosensing studies: Optical spectroscopy and Multivariate Analysis

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The main demand to establish an effective treatment against infectious diseases, which are responsible for most of the current health problems, are the correct diagnosis of the etiological agent and/or disease. Studies on biosensors has gain great visibility and applicability in the last few years due to its high selectivity and sensibility associated with non-evasive procedures to diagnosis. An interesting alternative to disease diagnosis has been reported in the literature, the study of biological materials by using optical spectroscopy techniques. In this report, we explore the use of Fourier Transform Infrared (FTIR) spectroscopy as a potential tool to fast identification and differentiation of different biological materials, such as, blood serum and bacteria. The spectrum of different samples was collected by in the range of 4000 to 600 cm^{-1}. The data analysis was performed by Principal Component Analysis (PCA's) and discriminative tests, such as Support Vector Machine (SVM) and k-Nearest Neighbor (K-NN). Our results showed that appropriated discriminative tests can reach 90% accuracy. The results suggests that this discrimination approach would be useful in a number of clinical scenarios where fast detection can improve the treatment sucess, and also it opens the possibility to new studies in the area to disease diagnosis.

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I17. Protein based Biomaterials from Biocatalysis to Photonics

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Protein's play as God in the biological system since they perform duties from generation, operation to the destruction of life by changing their form with fine tuning of amino acid sequences. While, perfect bio-mimicking of their functions seems impossible, it is possible to transform them into new biomaterials by changing their conformation for desired application. In this talk I shall be presenting my work on protein-based biomaterials developed for applications including biocatalysis and photonics. I shall be highlighting the fact that how by changing the secondary structural conformation of proteins *in vitro* can result in a new material desired for specific application.

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I18. Raman Imaging in SERS Studies

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Nowadays, metal nanoparticles are the basis for a number of devices coming from nanotechnological approaches that are expected to increase in near future. Among these technologies, those based on surface-enhanced Raman scattering (SERS) have been recently used with acute relevance. Although the SERS effect was itself discovered during the 70s, this spectroscopic method is benefiting from the unprecedented progress observed in the last few decades in instrumentation and materials development specific to nanoscale science. Indeed, the design of SERS active nanomaterials is a key aspect in further exploitation of SERS in diverse areas, including medicine, environmental monitoring and trace chemical analysis.[1]
The current developments of techniques such as Raman imaging, through high resolution Raman mapping with short measurement times, have brought a new look on composites and its applications. Such an image can show either the chemical heterogeneity or a specific response as SERS activity[2] or a labelling process (Figure 1). In this communication, our latest results in the development of SERS active substrates will be presented together with its evaluation using Raman imaging. Illustrative examples of SERS applications will be provided along with perspectives of development in chemical detection applied to real contexts. For example, SERS and Raman imaging were used with advantage in the monitoring of textile fiber dyeing.[2] Raman imaging allowed to explore the Ag distribution on the textile surface and to its interior, together with the study of the dye adsorption molecular species. Textile fibres containing Ag nanoparticles have been widely explored for antimicrobial fabrics. This investigation allows to foresee the use of this technique in terms of quality control of Ag containing fabrics, which is a market in great expansion.

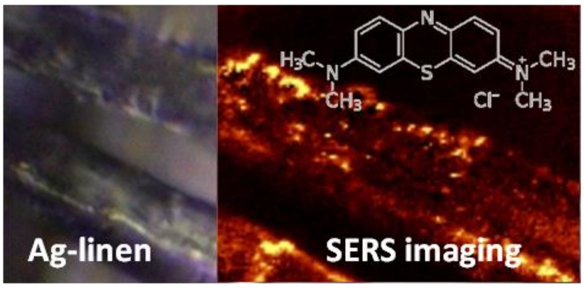

Fig. 1: Optical photograph (left) and Raman image (right) of a silver containing textile fibre dyed with methylene blue (chemical structure shown).

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I19. Computer Simulations: the Ultimate Tool to Understand Nanotechnology Experiments

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Computer modelling has become a fundamental tool to understand, rationalize and predict new materials. For almost 20 years, we have applied and developed computational models to complement complex experimental problems on nanomaterials. We will discuss, from the experimental point of view and in a non-technical manner, the most relevant computational models for nanotechnology. This will be illustrated by examples from our past and recent studies supporting experiments on carbon nanomaterial as well as in magnetic graphene [1], covalent organic frameworks [2] and inorganic nanoparticles [3].

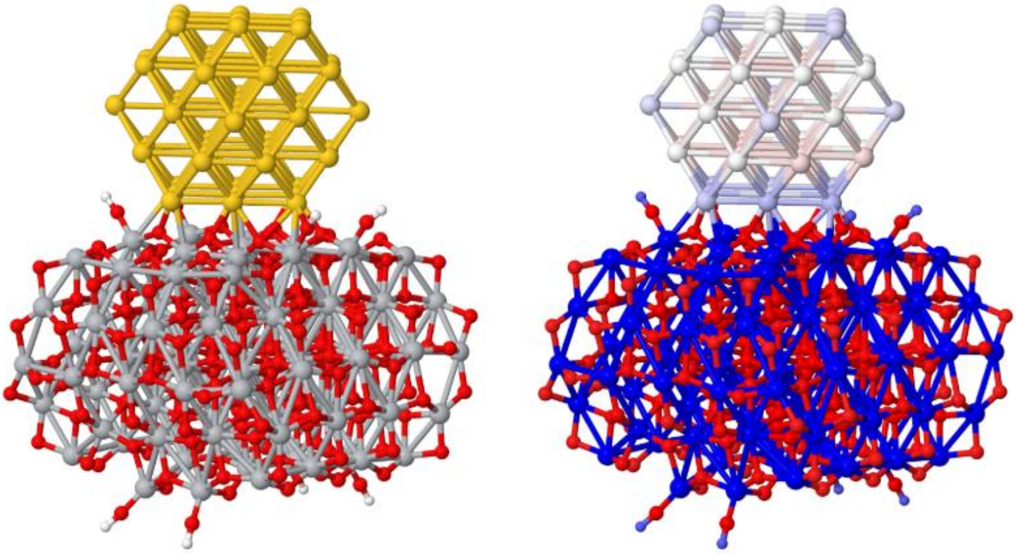

Figure 1. Gold nanoparticle adsorbed on a Titania nanoparticle in water, structure (left) and charge transfer (right) [3].

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I20. Chemical Solution Deposition of $BiFeO_3$ Films with Layer-by-Layer Control of the Coverage and Composition

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$BiFeO_3$ (BFO) is one of the perspective multiferroic thin-film materials because of its high spontaneous polarization and anti-ferromagnetic properties [1,2]. Chemical solution deposition (CSD) sintering technique allows to prepare large-scale thin films for the implementation in devices. In order to achieve films with several hundred nanometer thickness, the layer-by-layer deposition is usually used. Nevertheless, the role of the coverage and quality of the individual layers in the overall properties of the films is rarely discussed. In this contribution, we implemented piezoresponse force and conductive atomic force microscopies to study the layer-by-layer sol-gel deposition of BFO thin films focusing on the local phase distribution, morphology, piezoelectric response, and leakage current. The final properties of resulting thin films are found to be determined not only by the composition of the gel and crystallization step but by the gelation step as well. The drying temperature and treatment duration of the solution are shown to drastically influence the film coverage, which finally determines the morphology of the film and behavior of the crystallization process.

The equipment of the Ural Center for Shared Use “Modern nanotechnology” UrFU was used. The research was funded by Russian Science Foundation, grant number 19-72-10076.

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I21. Donor- and transition metal-substituted $SrTiO_3$: Relevant issues in the development of ceramic components for SOFC anodes

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Due to phase stability requirements, the choice of alternative perovskite-type materials for ceramic SOFC anodes is essentially limited to chromite-, molybdate-, vanadate- or titanate-based systems. Donor-doped $SrTiO_3$ combines remarkable stability in both oxidizing and reducing conditions, substantial electronic conductivity, and good prospects for inhibition of carbon deposition and sulfur-tolerance.

The present lecture gives a brief overview and a comparative assessment of a variety of strontium titanate-based solid solutions as fuel electrode materials with emphasis on the defect chemistry, reducibility and corresponding effects on the electrical properties, thermomechanical compatibility with solid electrolytes, and electrochemical activity. The exemplified oxide systems are $(Sr,Ln)TiO_3$ (Ln = La-Yb), $(Sr,Pr)TiO_3$, $Sr(Ti,Ta)O_3$ and $Sr(Ti,V)O_3$ series including nomically cation-stoichiometric and A-site deficient formulations [1-4].

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I22. GaTe melt grown single crystals for optoelectronics: solid state phase transitions, structural defects, optical propertries

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Gallium telluride is a typical representative of AIIIBVI semiconductor compounds known for their optical and electric properties, which make them applicable for using in electronic and optoelectronic devices. Some properties of gallium chalcogenides are similar to those of traditional semiconductors (for example, the energy gap is in the range 1-2 eV, like in silicon). However, their layered structure and direct energy gap, which can be engineered through changing in a film thickness and a doping concentration, make them even more attractive for optoelectronic applications. As regards crystallographic structure of GaTe, it makes exception in the group of AIIBVI crystals. In stable state, it crystallizes in monoclinic phase. In some cases monoclinic phase transforms into hexagonal and vice versa, but this concerns only thin films and is ascribed to size effect. From preliminary synthesized compound of stoichiometric GaTe obtained from pure 6N Ga and 5N Te we had grown from melt GaTe single crystal using high pressure vertical zone melting under 100 atm of Ar pressure at a pulling rate 9 mm/h as described in [1]. The crystal was of 20 mm in diameter and 70 mm in length. Its structure was studied using an URS-2.0 set up with a copper anode and RKSO camera. XRD was used for phase analysis and EPMA for elemenal analysis. Vickers microhardness data and transmission optical spectra in IR and visible ranges are provided.

The polymorphic transition goes as a non-variant process at a constant temperature and pressure without any changes in composition. The single crystalline structure is preserved after the transition, despite the process being diffusive. This is due to presence of the coherent boundary between two phases, which is a cleavage plane transforming from (0001) in hexagonal phase to $(\bar{2}01)$ in the monoclinic. Annealing of the transformed monoclinic GaTe at 1023K followed by quenching does not incite decomposition of the compound, which is explained by high stoichiometry of the grown crystal. Energy gap value after storage at room temperature and after the annealing is 1.65 eV, which corresponds with the data for monoclinic GaTe. The Vickers microhardness is 360 MPa.

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I23. Multiscale modeling of multilevel memory elements as synapses necessary for creating neuromorphic networks

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The design and optimization of memristive elements is based on an understanding of the processes of formation of conducting channels, knowledge of the detailed switching mechanisms between the various states of the memristor. In this regard, mathematical models play a significant role, making it possible to obtain detailed pictures of the ongoing processes. The complexity of creating models of this class is associated, first of all, with the need to take into account a wide range of spatio-temporal scales, which makes the application of multiscale modeling technology relevant.

To solve the problems of multiscale modeling, in this work, we used the author's information technology for constructing multiscale models based on the set-theoretic representation of physical and mathematical models and the use of information structures that combine data and processing methods. On its basis, an original architecture of a high-performance software complex has been developed, which allows for effective parallel solving problems from different scales, taking into account the constant exchange of data. A mathematical model of the formation / destruction of conducting channels (filaments) in memristor elements based on oxide films was built, including 5 interconnected submodels. To directly study the thermodynamics and kinetics of the processes of formation / destruction of conducting channels (filaments) in memristor elements based on oxide, a thorough analysis of a set of semi-empirical methods potentially suitable for this purpose was carried out. For a systematic consideration of the thermodynamic driving force of the origin of possible types of defects, a large-scale molecular dynamics simulation was carried out with the selection of suitable interatomic interaction potentials with identified parameters.

This work was supported by the Russian Foundation for Basic Research, project No. 19-29-03051 mk.

I24. Growth of Few layered 2D materials by Chemical Vapor Deposition

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Oflate, research is centered on Two-dimensional (2D) materials owing to their tunable electronic, optical, and chemical properties in addition to the abundant choice of materials available. Furthermore, 2D materials based heterostructures prepared by combination of materials offer exotic properties as well as novel applications. To realize this large area films are required and in this context chemical vapour deposition (CVD) is a powerful method. Over the years, chemical vapour deposition (CVD) has been extensively used to grow 2D materials and their heterostructures in recent years, despite several challenges still remain.

In this talk, insight's into the large area growth of ReS2 on different substrates is provided. The growth of MoS2 on large area is also deliberated. Solutions to these challenges and ideas concerning future developments in this emerging field are discussed.

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I25. Fabrication of BCZT piezoelectrics for energy conversion

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Piezoelectric oxides are one of the key areas of research due to their beneficial applications in fields such as sensors, actuators, transducers, microelectromechanical systems, energy storage. Recently lead-free piezoelectrics have gained application potential in refrigeration and energy storage. Current vapour based air-conditioning and refrigeration technologies contribute directly or indirectly to a significant global electricity consumption. Hence development of high quality environmental friendly piezoelectrics is vital for applications.

(Ba,Ca)TiO3-Ba(Ti,Zr)O3 (BCZT) solid solutions at the morphotropic phase boundary is one of the highly reported piezoelectrics for devices. Compositional control of BCZT is crucial for optimal piezoelectrics at micro/nano-scale. In this study we report on the growth of BCZT fibre crystals as well as thick and thin films following laser-material interactions. By means of chemical and physical deposition techniques various BCZT piezoelectrics are fabricated for ferroelectric and electrocaloric studies. We observed improved physical properties in thin and thick films compared to the literature while the fibre crystals have compositional heterogeneities

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I26. Flexible piezoelectric biomaterials for sensors

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Piezoelectric actuators, sensors and nanogenerators are key enable technologies for the so called "Internet of Thing". Recently, actuators and sensors are being implemented in different applications for healthcare, enlarging the concept to "Internet of EveryThing". Based on this, it is desirable the flexibility and biocompatibility of materials for close interaction with the body. This work describes the preparation of piezoelectric bionanocomposites composed of lead-free barium titanate nanoparticles within a biopolymer matrix. Chitosan, which is a polysaccharide with the ability to generate films, gives the biopolymeric flexibility, while the barium titanate assigns the ferroelectric and piezoelectric properties. The addition of barium titanate particles improved the mechanical properties of the chitosan films, making them more resistant, elastic and ductile. These films were more resistant to water than pure chitosan films, revealing the interaction between the particles and the chitosan matrix. In relation to the electric behavior of the films, the increase of particles improves the permittivity of the samples five times in relation to the biopolymer material. For comparison reasons, bionanocomposites with alginate and starch matrices and the highest concentration of barium titanate were also prepared in order to evaluate the polysaccharide nature effect on the piezoelectric properties. The piezoelectric response force microscopy of these films was performed, and the results will be discussed.

Acknowledgment: 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 FCT/MEC and when appropriate co-financed by FEDER under the PT2020 Partnership Agreement; NANOTRONICS (IF/300/2015); FLEXIDEVICE (PTDC/CTM-CTM/29671/2017). This work was also funded by national funds (OE), through FCT, in the scope of the framework contract foreseen in the numbers 4, 5 and 6 of the article 23, of the Decree-Law 57/2016, of August 29, changed by Law 57/2017, of July 19.

I27. Effect of Disorder on the Metal-Insulator Transition of Vanadium Oxides by Soft X-Ray Irradiation

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Photocontrol of the conducting phases for transition metal oxides is important for the development of sensors and data storage devices. VO_2 and V_2O_3 are both prototypical materials with easily accessible metal-to-insulator transitions (MIT) 348 K and 165 K, respectively and co-occurring structural phase transition (SPT) [1]. These effects have posed long-standing theoretical questions [2]. Even the most fundamental issue, whether the microscopic mechanism which results in the MIT is due to short-range (“local”) or long-range (“global”) correlations, is under debate. An example of global correlations is the appearance of long-range order (magnetic or structural), which doubles the unit cell. This in turn opens up a gap at the Fermi surface of a half-filled metallic band [3], giving rise to the MIT. The more local correlations giving rise to the MIT arise from competition between the kinetic energy, which favours electron transport, and the Pauli Exclusion Principle, which inhibits electron hopping [4]. Small amounts of disorder tend to disrupt long-range electronic correlations but have only a minor effect on the local ones. This allows probing of whether global or local correlations drive the changes in conductivity.

We show that the soft x-ray irradiation can induce the metal-to-insulator transition at room temperature in two similar systems; V_2O_3 and VO_2 thin films grown on *R*-plane sapphire. The ability of soft x-rays to induce oxygen desorption in both of the thin films are confirmed by photoemission and x-ray absorption spectroscopy, which also revealed the strikingly different effects of irradiation on the two materials. Soft x-ray irradiation was found to induce a lasting increase in conductivity of VO_2 and V_2O_3 thin films. Analysis of valence band photoemission spectra revealed that the density of states (DOS) of the V 3*d* band increased with irradiation time, while the DOS of the O 2*p* band decreased. We use the observations from soft x-ray spectroscopy to propose a model that the irradiation driven metal to insulator transition in both vanadium oxides is due to oxygen desorption. The results may direct the way toward the development of new routes for controlling the conductivity of V_2O_3 and VO_2 thin films by light.

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I28. Catalyzed magnesium hydride for clean energy storage applications

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As we approach the end of the hydrocarbon era, clean energy demands are increasing and options such as hydrogen, heat and electricity gain higher importance. Interestingly, all these three energy carriers can be derived from solar power and used for propelling automobiles and household devices. Nonetheless, only when a high density energy storage option is established our clean energy harvesting trials become a practical reality. In this context solid state materials receive attention as energy storage materials and the authors believe that presently Mg is the best reversible material for storing large amounts of hydrogen, heat and electricity. Mg reversibly stores 7.6 wt.% hydrogen as per reaction (1) which is higher than the USDOE target of 5.5 wt.% H_2 for vehicular applications [1].

$MgH_2 \leftrightarrow Mg+H_2$ (1)

For reaction (1), the equilibrium dehydrogenation at 1 bar occurs at ~300 °C. The forward reaction is endothermic and the reverse reaction is exothermic with a heat involved in the reaction is 74 kJ/mol. It means, ~2800 kJ/kg heat energy is absorbed into the Mg-H system during every dehydrogenation cycle and the same amount is released during every hydrogen charging cycle. This huge amount of heat can be used for converting water to steam which apparently can be used to operate a turbine for producing electricity. MgH_2 can also be involved in an electrochemical reaction with Li as per the reaction (2)

$MgH_2+2Li \leftrightarrow Mg+2LiH$ (2)

Interestingly, when deploying MgH_2 as anode for a Li ion battery, it can reversibly deliver 2038 mAh/g capacity which is more than five times higher than the electric energy delivered by carbon anodes. The information existing in reactions (1) and (2), therefore clearly conveys the fact that Mg is a rare material with property to store multiple forms of energy; hydrogen, heat and electricity, in large quantities. However, to make MgH_2 effectively involved in (1) and (2), the Mg-H sorption interaction kinetics should be fast enough but the high activation energy (153 kJ/mol.H_2) of as-received samples present a significant challenge by making diffusion barriers. Our research reveals that by using metal oxide additives [2] with Mg/MgH_2 the activation energy can be significantly reduced which apparently improves the suitability of Mg for storing hydrogen, heat and electricity. Especially by using Nb_2O_5 as additive we observe that the activation energy can be reduced to 100 kJ/mol. As it improved the system efficiency a many fold we are currently interested in identifying most suitable additives through which we can reach out to breakthrough observations for storing hydrogen, heat and electricity.

Acknowledgement

Pukazh acknowledges financial support from FCT (Portugal) with references, CENTRO-01-0145-FEDER-022083 and CEECIND/04158/2017.

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Oral presentations

O1. Properties of $Mg_{2-x}Al_xNi$ (x = 0, 0.1, 0.2, 0.3) alloys prepared by mechanical alloying for electrochemical hydrogen storage

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In this work, we synthesized Mg_2Ni alloys with a magnesium substitution by another element which is Aluminum (x = 0, 0.1, 0.2, 0.3) by ball milling. The effect of the ball-milling on the alloy structure and surface image was examined by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The TEM. XRD analysis results indicate that Al substitution can interstitially dissolve hydrogen atoms.
These alloys used as negative electrode in nickel-metal hydride batteries have been studied by different electrochemical techniques. Several methods, such as, galvanostatic charge /discharge cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS). The $Mg_{1.8}Al_{0.2}Ni$ alloy achieved maximum discharge capacity is about 120 mAh/g.

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O2. Metal Halide Perovskite Nanomaterial and MOF Composite Thin Film electrode fabrication using commercially available inkjet printer

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Metal Halide Perovskite are excellent semiconductors, finding applications in low-cost, high-efficiency opto-electronics and photovoltaic devices technology. Main problem associated with them is the stability in ambient atmosphere. On the other hand, Metal organic frameworks with good structural tailor ability, excellent chemical and thermal stabilities, large surface area and tunable pore size. These phenomenal characteristics motivate researchers to utilize MOFs as favorable template for host- guest chemistry with the Hybrid halide perovskite. In this work, we synthesize methyl ammonium lead bromide perovskite composite with MOF-5 (Zn-MOF) by simply inkjet printing the MOF Inks on to different substrate and then loading the CsPbBr3 and MAPbBr3 perovskite precursor salts into these printed films using dip coating approach. Incorporated perovskite MOF composite showed high luminescent at 527nm with excitation on 360nm nature with great amount of stability in the ambient atmosphere for months.

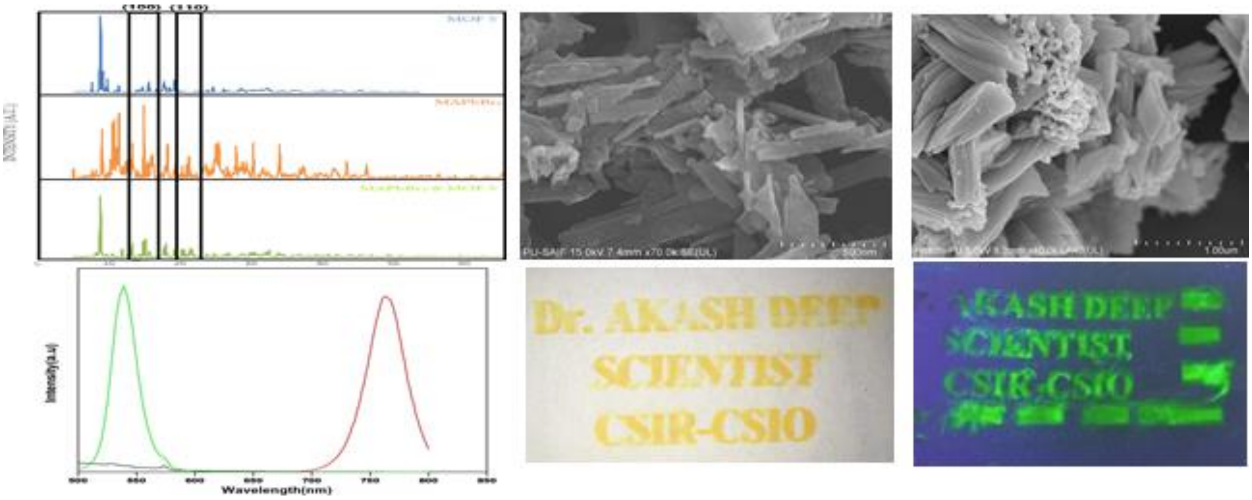

Figure 1 (a) XRD spectra and (b) SEM Image of Cu-MOF and MAPbBr3@CuMOF. (d)PL spectrum of the Pb MOF, MAPBBr3 and MAPbI3, Inkjet Printed pattern of (e) MAPbBr3@MOF(Visible) (f)MAPbBr3@MOF(UV)

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O3. Chemical Reduction of Toxic Pollutants from Water Environment by Rod-like Silver Coordinated Melamine based Polymer

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Substantial flourishment in the chemical industries involving the manufacturing of dyes, pharmaceuticals, plasticizers, various industrial solvents, and explosives has led to the hazardous release of nitroaromatic effluents in the environment causing an immense detrimental effect on the aquatic ecosystem [1]. Among all nitroaromatic pollutants, 4-Nitrophenol (4-NP) deserves extensive treatment owing to its carcinogenic, mutagenic, non-degradable and toxic nature [2]. One of the effective remediation methods includes chemical reduction of 4-NP to non-toxic and easily degradable compound 4-Aminophenol(AP). The present work involves the facile synthesis of a Silver-Melamine (Ag-M) based coordination polymer and its subsequent utilization in effectively degrading different toxic pollutants specially 4-NP. Ag:M is taken in the molar ratio of 1:2 which when heated at 100^{o}C in an oil bath forms a stable white colored gel. The powder product is obtained after vacuum drying the gel at 50^{o}C. Detailed characterization techniques include XRD, FTIR, FESEM, and DRS which reveals the phase formation, nature of chemical bonds and the rod-like morphology of the sample. The as-synthesized sample exhibits superior degradation activity in reducing 4-NP to 4-AP in the presence of sodium borohydride ($NaBH_4$) within 6 minutes. Several variations of the parameters influencing the chemical reduction activity have been performed to study their effect on the reduction reaction. Chemical reduction activity increases manifolds by increasing the $NaBH_4$ concentration and also the Ag-M dosage. The optimum result has been obtained for 1 mg Ag-M dosage and 0.005M $NaBH_4$ concentration in degrading 0.001M 4-NP within 6 minutes. A plausible mechanism has been proposed to understand the chain of reduction reactions taking place. Moreover, the as-prepared Ag-M sample has been further utilized for degradation of textile dye Methyl Orange (MO) by the same procedure. The sample has shown impressive reduction results by completely degrading MO within 6 minutes in presence of a small concentration of $NaBH_4$. The novel Ag-M material thus proves to be extremely beneficial in degrading harmful dyes. This, in future, might establish its potentiality as a feasible material for waste water remediation.

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O4. Carbon nanoparticle-vesicles nanocomposites for biomedical applications

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Fatty acid or lipid vesicles are now-a-days becoming very good agent in biomedical research for their bio-mimicking characteristics. Such systems have already been used in many aspect like drug/gene delivery, nano-reactor etc. Here, we developed a hybrid system of fatty acid vesicles taking oleic acid as staring material and the carbon nanomaterial called graphene quantum dot (GQD). The so formed hybrid vesicles was successfully used to load drug (used methylene blue as model drug) and pH dependent drug release was observed. Drug loading was quite higher in hybrid vesicles (98.3%) compare to bare oleic acid vesicles (71.98%). Similarly, drug release was significantly higher for hybrid vesicles than the bare one and at pH 5, it gives more release than at pH 7.4. Apart from that we also prepared a nanohybrid system from palmitic acid vesicles and (palmitic acid-cholesterol) carbon dot. Subsequently, it was used for uric acid (UA) and ascorbic acid (AA) absorption which act as prominent toxins in our body. Interestingly, the nanohybrid was found to be efficient UA absorber (~80%) compare to pure palmitic acid vesicles (~60%) confirming the role of carbon dot in absorption. Till now there is no report of toxin absorption by vesicles system. So, this will lead to an effective material for toxin removal from our body.

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O5. Adsorption of C_{60} fullerenes on metal-modified Si(111) surfaces

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There is a great abundance of the ordered metal/silicon reconstructions exhibiting a variety of structures and properties, they can be thought of as promising substrates for studying adsorption behavior of C_{60}. A set of research works on C_{60} adsorption on the most "popular" metal/silicon reconstructions were carried out. The primary method for surface research was scanning tunneling microscopy. The most important and relevant results of these studies are presented in this report.

We investigated adsorption C_{60} fullerenes on Si(111) surface covered by an atomic layer of Tl, Pb, or their compound and discovered a set of C_{60} nanostructures that appear to be constructed using a universal building block made of four C_{60} molecules. Given the unique properties of the substrate, these nanostructures promise to be two-dimensional nanostructured superconductors whose properties are awaiting their exploration [1].

Having studied the formation of ordered quasi-one-dimensional structures from straight chains of C_{60} fullerenes on (Au, Tl)/Si(111) system, our group obtained important structural information that may be useful for the prospective works on elucidating the ways to control electronic properties of the Si(111)5×2-Au surface using atomic and molecular adsorbates [2].

Exploring the (Tl, Au)/Si(111)7×7 compound reconstruction, we have found that C_{60} fullerite film shows up as a proper capping layer for it. Due to a perfect non-distractive epitaxial C_{60} overgrowth, the metallic Tl-Au compound preserves at the deeply buried interface its atomic structure and all basic electronic properties [3].

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O6. Properties of lightweight aggregates obtained from clay and spent zeolitic adsorbents

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This work presents results of research on the possibilities of using waste in the form of used zeolitic sorbents (NaP1 and clinoptilolite) after sorption of petroleum products as components modifying the properties of sintered ceramic material in the form of lightweight aggregates (LWAs).

To this end, physicochemical, mineralogical and structural properties of used materials were determined, raw material mixture of clay and waste was prepared which was subjected to the sintering process. The effect of modifiers on final properties of obtained LWAs was determined. Physical and mechanical parameters were estimated using standard methods (EU-EN-13055-1). Structural characterization of raw materials and LWAs was made using X-ray diffraction (XRD), scanning electron microscopy (SEM), mercury intrusion porosimetry (MIP) and X-ray computational microtomography.

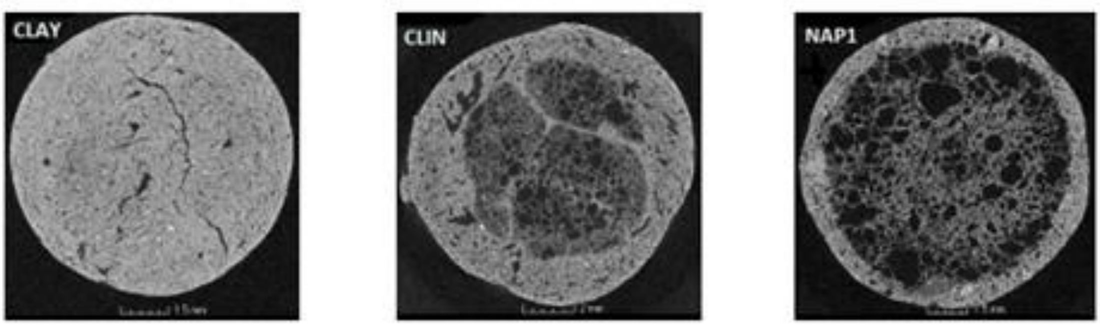

Figure 1. Exemplary 2D cross-sectional images derived from microtomography for the studied materials. Black areas: pores; white areas: solid

The addition of waste zeolites has fostered a decrease in the particle density, which in turn has involved a decrease in the mechanical resistance. A decrease in water absorption also occurred. The pore structure of LWAs prepared from a clay deposit was strongly modified by the addition of spent zeolites, depending on the composition of the starting mixture. The reuse of the zeolitic sorbents containing petroleum waste to produce LWAs leads to advantageous properties of the resulting LWAs indicating their applicability in geotechnics, building construction and agriculture.

The research was financed from statutory funds FN14/ILT/2019.

O7. Scratch resistance and morphological analysis of CrN and DLC coatings on duplex treated X42Cr13 plastic mould tool steel

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The paper deals with the characterisation of surface mechanical response of two different ceramic coatings – DLC and CrN – deposited on X42Cr13 plastic mould tool steel under increasing normal load during instrumented scratch test. The aim of the study is to analyse the effect of duplex treatment, surface preparation and coating material on the failure mechanism and degree of damage of the coated material system, in addition to characterize the scratch resistance by the critical normal load and the friction coefficient at the failure of coatings. Hardness and VIF toughness tests were accomplished to compare the resistance of the coatings to static compressional loading, furthermore to define the adhesion strength and work needed to remove the coating from the substrate. Morphological analysis of the scratch tracks was accomplished using optical and scanning electron microscopy. The most important results of the research work are as follows:

- Duplex treatment can improve efficiently the scratch resistance of the coated plastic mould tool steel;
- Scratch morphology and quantitative characteristics of the scratch resistance strongly depend on coating material, heat treatment condition and surface preparation of the substrate.

Based on the obtained results performance of the coated material systems can be improved efficiently.

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O8. Synthesis, Structural, Tribological and Magnetic characterization of Double doped Strontium Bismuth Niobate Lead free ceramics

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The $SrBi_2Nb_2O_9$ (SBN), $SrBi_{1.8}Pr_{0.1}Gd_{0.1}Nb_2O_9$ (SBPGN), $SrBi_{1.8}Eu_{0.1}Gd_{0.1}Nb_2O_9$ (SBEGN) and $SrBi_{1.8}Eu_{0.1}Y_{0.1}Nb_2O_9$ (SBEYN) double-doped ceramics were prepared from two-stage Solid-state reaction method. The prepared samples have been subjected to Powder X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Fourier Transform Infrared Spectroscopy (FTIR), Tribological and Vibrating Sample Magnetometer (VSM) studies. From the TG/DSC study on SBN, optimized temperature of material formation has been identified and is found to be above 1100^0C . The density of sintered ceramic samples (1120^0C for 2hr) was measured from Archimede's principle. The percentage density of the studied ceramic materials has been identified to be in the range of 94-95%.The crystal structure was obtained by XRD technique, which established single-phase crystal structure in all the studied samples. The lattice parameters have been obtained using POWD software. The morphological study of the samples was conducted employing SEM. The SEM studies have resulted in plausible needle shaped grains in SBN, SBPGN, SBEGN and SBEYN with induced porosity being 1.99µm, 1.34µm, 5.33µm and 2.20µm respectively. The EDS study necessitates the presence of individual elements in all the prepared materials. The changes in the vibrational modes with respect to pure material and double doped SBN materials have been understood interms of FTIR spectra. The tribological properties were realized through Vickers's Hardness, Wear Coefficient and Friction Coefficient studies on the samples. The VSM studies on the samples have revealed that magnetic properties are being inducted from double doping of Praseodymium – Gadolinium (PG), Europium – Gadolinium (EG) and Europium – Yttrium (EY) at Bi-site of SBN.

O9. Flame retardant finishing of cotton fabric based on Ionic liquid compounds containing boron prepared with the sol-gel method

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Cotton (CO) fabrics with flame retardant properties based on ionic liquids: 1-methylimidazolium chloride propyltriethoxysilane (MCPTS) and pyridinium chloridetriethoxysilane (PCPTS) with boron getting from boric acid are successfully obtained via a sol-gel process. Fourier transform infrared spectroscopy (FTIR), Optical microscopy analysis and scanning electron microscopy (SEM) images, were first carried out to characterize the chemical composition and the morphology of the treated and untreated cotton fabrics, respectively. The investigation of flame resistance was evaluated by the vertical burning test. It was observed that the treated cotton fabrics exhibited good flame-retardant properties and did not burn even after 10 (s) flame application duration and the rate of flame spread was inhibited compared to the pristine cotton fabric. Furthermore, the thermal comportment of cotton fabrics was performed by thermogravimetric (TG) analysis and differential scanning calorimeter (DSC). Moreover, the tensile strength of the treated textiles is mostly reserved. In this work, we prove that the sol-gel method using ionic liquids and boron could be used as an effective flame retardant, to develop finishing cotton fabrics for textile fireproof applications.

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O10. Preparation of X-type zeolite-carbon composite from fly ash and its application for petroleum products removal

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Fly ash (FA) belongs to the group of industrial wastes which are annually produced in very large quantities (800 Mt). It is estimated that only ¼ of annual FA production is utilized, mostly as a raw material for cement synthesis and construction materials. One of the problematic aspect limiting the FA utilization is the type of ash with high carbon content.

The aim of this work was to obtain new type of zeolite-carbon composite (NaX-C) from fly ash with an increased content of unburned carbon (around 40%), characterization of its physicochemical properties and assessment of sorption capacity towards petroleum substances.

Structural characterization of raw fly ash and NaX-C was made using X-ray diffraction (XRD), scanning electron microscopy (SEM). The textural parameters were determined using nitrogen adsorption/desorption isotherms at liquid nitrogen temperature. Adsorption capacity towards engine oil was determined gravimetrically using Westinghouse method.

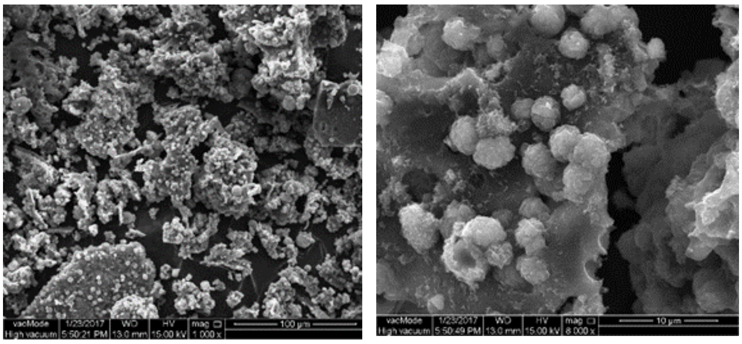

Figure 1. SEM images of the NaX-C composite.

SEM analysis revealed that well-defined zeolite crystals were formed on porous carbon aggregates. The specific surface area S_{BET} of the composite was 230 m²/g. Adsorption capacity towards engine oil was 150%.

The resulting composite material can be applied as an effective adsorbent for petroleum spillages removal. Due to its organic-inorganic nature, relatively low cost of obtaining and physicochemical properties it is also expected to be used as multifunctional adsorbent and ion-exchanger.

The research was financed from statutory funds FN12/ILT/2019. Lidia Bandura was supported by the Foundation for Polish Science (FNP).

O11. ZnO-nanorods grown on flexible substrate for selective host peripheral blood mononuclear cells immobilization

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This work reports the selective isolation of Natural Killer cells from whole peripheral blood mononuclear cells (PBMC) using the vertically aligned ZnO nanorods on a flexible ITO (indium tin oxide) coated PET (polyethylene terephthalate) substrate by using electro-deposition technique. These ZnO nanorods were characterized by using various techniques like X-ray diffraction (XRD), Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM), Photoluminescence (PL), Fluorescence Life Timeimaging Microscopy (FLIM). XRD and TEM confirmed the wurtzite (hexagonal) structure of ZnO nanorods. The use of this ZnO nanorod-immunoaffinity based platform allows the isolation of NK cells from PBMC samples. The obtained crystallanity of well-aligned ZnO nanorods (NRs) proved its efficiency in immobilizing the monoclonal anti-human NKp30 antibody (mAb). This design obviated additional procedures for mAb immobilization. The successful selection of NK cells from PBMCs by our nanoplatform, was assessed by the photoluminescent properties of acridine orange together with these cells' activation via B7-H6. This easy and straightforward ZnO-mAb nanoplatform paves the way for the design of biosensors for clinic diagnosis, and/or due to its inherent biocompatibility, for the selection of PBMC aiming transplantation therapies.

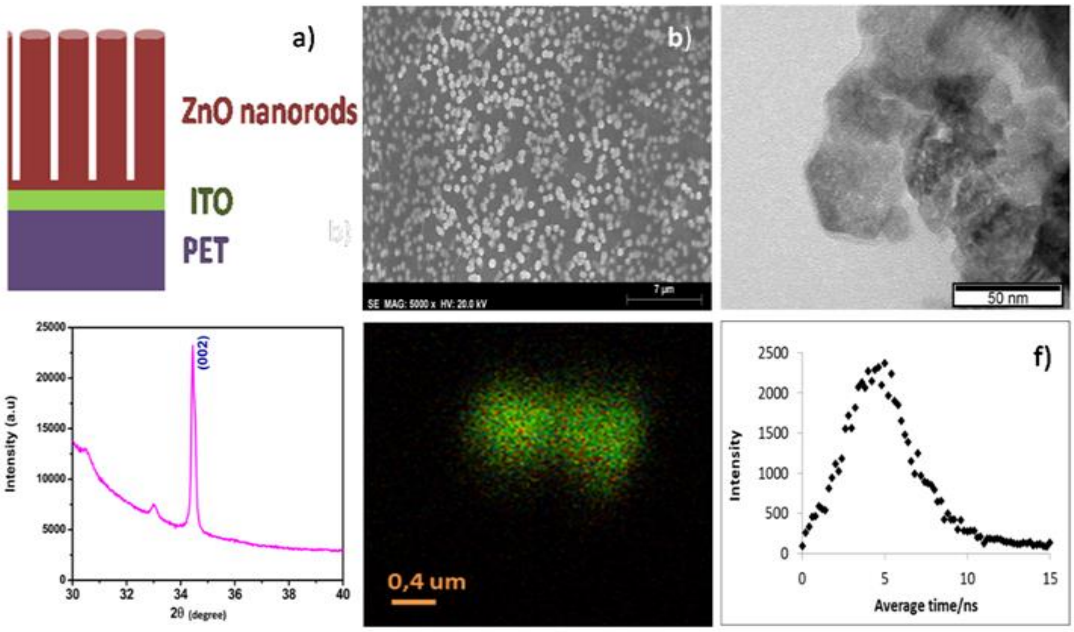

Fig. 1

O12. Statistical tolerance analysis of flexible assembly taking into account spot welding effects

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Tolerance analysis of flexible parts and assemblies is the precious step in manufacturing parts in industry, in order to minimize the cost of the process. During the assembly process, the spot-welding effects are inevitable. It causes form deviations of the final assembly. The aim of this paper is to analyze tolerances in assemblies of flexible parts taking into consideration form deviations of parts and spot welding effects. The Influence Coefficient Method is used for calculating the final deviations of the final assembly. In this case, errors in each part are assumed to have a statistical distribution. Finally, through an example, the results prove the performances of the proposed approach.

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O13. The effect of the addition of synthetic zeolites on the hydration of alite

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Alite is the main component of cement clinker. In the aquatic environment, it is hydrated, as a result of which is the C-S-H phase. The C-S-H phase is mainly responsible for the properties of hardened cement paste. To increase the efficiency of cement hydration, various pozzolanic additives are used. They modify the phase composition of the hardened paste by reducing the amount of $Ca(OH)_2$ portlandite and by changing the CaO / SiO_2 ratio in the C-S-H phase. That positively affects the properties of the cement paste.

Zeolite minerals are increasingly used as pozzolan minerals used in the production of cement and concrete. Zeolites are a group of hydrated aluminosilicates with adsorption, catalytic, ion exchange and pozzolanic properties. In order to determine the effect of the addition of these minerals on the hydration process of allite, three structural types of zeolites were selected: Na-A, Na-X, and ZSM-5. Zeolites had a different Si / Al respectively; 1.0; 1.2; 77.0.

All synthetic zeolites were obtained by the hydrothermal reaction of the waste solution formed after the synthesis of zeolites from fly ash with calcium hydroxide. Alite was synthesized in the laboratory from a mixture of CaO and SiO_2 in a molar ratio of 3: 1 with an admixture of 1.5% by mass MgO and 0.8% by mass Al_2O_3. The quantitative content of zeolites and alite determined by the Rietveld method was> 98%. Such high purity of materials significantly reduced the impact of other mineral components commonly found in cement (Ca_2 [SiO_4] - belite, Ca_3[Al_2O_6] - tricalcium aluminate and C_2 [AF] - ferrite) on their hydration.

In order to determine the effect of the addition of zeolites on the hydration of alite, pastes were prepared in which the quantitative share of individual structural types of zeolites was 15%, 30% and 50%. Tests carried out using scanning microscopy (SEM) after 3, 28 and 90 days of sample conditioning showed a significant difference in the morphological structure of the slurries. As the slurry ripened, the transformation of the C-S-H phase from a compact gel into a honeycomb mold was observed.

X-ray phase analysis (XRD) showed that the addition of 15% caused an increase in the C-S-H phase content at the expense of the quantitative share of portlandite. These samples were characterized by a compact structure. On the other hand, the replacement of 50% of the alite with zeolites, in each case caused a loss of compactness of the obtained slurries and an increase in the content of $Ca(OH)_2$. Clear differences in the phase composition of slurries were observed as a result of the use of different structural types of zeolites. The largest quantitative share of the C-S-H phase was recorded for ZSM-5 zeolite, which has the highest Si/Al ratio. The addition of ZSM-5 accelerates the hydration of alite, regardless of the amount of zeolite in the grout. In contrast, for Na-A and Na-X zeolites, acceleration is only visible for 15% of their addition.

The study confirmed the hypothesis that the structure of zeolite affects the type of hydration products formed.

The research was carried out as part of the TEAM-NET project – POIR.04.04.00-00-14E6/18-00 financed by Foundation for Polish Science

O14. Structure and Luminescent Properties of Cyan emitting Eu^{2+}-doped $BaAl_2O_4$ Nanophosphors

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Nowadays Solid-state lighting (SSL) replaces conventional lighting sources such as incandescent bulbs and fluorescent tubes [1]. White light-emitting diodes (w-LEDs) have gained much attention as the next generation source of lighting owing to its long lifetime, high energy efficiency, short response time, environmental friendliness, energy savings and material hardness [2]. Highly luminescent cyan emitting Eu^{2+} doped $BaAl_2O_4$ nanophosphors were synthesized by simple sol-gel method. The structural and optical properties of the cyan emitting nanophosphors were investigated by using the X-ray powder diffraction (XRD), Rietveld refinement of XRD, Field Emission Scanning Electronic Microscopy (FESEM), UV- Visible spectroscopy and Photoluminescence spectroscopy (PL). The as prepared nanophosphors emits strongly in the blue-green (cyan) region of 490 nm under 350 nm UV excitation. The photoluminescence emission intensity and the color brightness of the nanophosphors enhances with the increase in Eu^{2+} doping concentration and quenches at a certain percentage of Eu^{2+} ion. The developed nanophosphor shows brighter cyan emission due to the enhancement of defect states inside the host matrix. Color purity is also higher for the doped samples due to the lowering of the the nonradiative transition centers in it. Obtained results indicate that $BaAl_2O_4:Eu^{2+}$ is a promising cyan emitting nanophosphor for white light LEDs.

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O15. Amino terephthalic Acid Functionalized Graphene Electrode For Impedimetric Immunosensing Of *E. coli*

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Graphene oxide (GO) has been functionalized with 2-aminoterephthalic acid, followed by the exploitation of this functional material for the development of an electrochemical immunosensor for *E. coli* (*Escherichia coli*). The application of 2-aminoterephthalic acid for the functionalization of GO is fairly simple, and the success of the method has been proven with the help of different instrumental characterizations. The proposed antibody-based biosensor has exhibited a wide range of detection capability (2.2×10^2 - 2.2×10^8 cfu/mL) with very low limit of detection, of 2.2 cfu/mL. The present sensing system also offered a fast response time (4 minutes), stability (up to 2 month) and reproducibility. The analytical performance of the prepared biosensor was comparable to most of the previously reported electrochemical biosensors for *E. coli*. As such, the herein proposed novel yet simple approach of functionalization of graphene should be useful to allow the development of other similar sensing systems for other environmentally and clinically important analytes.

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O16. Tolerance analysis of mechatronics systems

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Mechatronic systems appeared to meet new requirements in terms of performance, comfort, safety and consumption. However, the design of these systems remains a real challenge despite the new methods. In fact, the multidisciplinary of these systems leads to considering innovative solutions. To optimize the tolerances taking into account construction uncertainties of components that can lead to considerable degradation of system performance. So the consideration of these uncertainties in the design and sizing phase must make it possible to limit and above all to anticipate this deterioration. In this article, a new approach has been studied that allows the analysis of mechatronic system tolerances. This approach is based on Monte Carlo method. To illustrate our approach, we treated an example of a robotic arm.

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O17. Electrical Transport Properties of Nickel Nanoparticles

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Magnetic nanoparticles (NPs) attract much attention in research due their superior multifunctional properties, which are significantly deviated compared to their bulk counterpart, mainly due to increase in grain boundaries, larger fraction of atoms on particle surface and modification in electronic density of states [1]. Among others, Ni NPs show many applications in optics, catalysis, high-density magnetic recording media and base-metal-electrode multilayer ceramic capacitor, due to their good magnetic, electrical and thermal properties. Particularly, electrical transport properties of metal NPs highly depend upon particle size, shape and surfactant/s used during synthesis. Solution phase synthesized Ni nanoparticles (NPs) of Scherrer size 20.5 ± 0.4 nm are characterized systematically using X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM) and X-ray photoelectron spectroscopy (XPS). Their electrical transport properties in temperature range 5 K to 300 K are studied using electrical resistivity (ρ) and Seebeck coefficient (S). The ρ and strength of electron-phonon interaction ($\alpha_{e\text{-}ph}$) are increased while residual resistance ratio (RRR) and Debye temperature (θ_D) decreased in NPs compared to bulk Ni. Furthermore, an unusual crossover from negative to positive S, and suppression and shift at higher temperature in phonon drag feature for NPs compared to bulk are observed. These results are mainly attributed to confinement of electrons and phonons and their enhanced scattering from grain boundaries and other defects.

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O18. Temperature and time controlled synthesis of instable vaterite microparticles

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Calcium carbonate ($CaCO_3$) exists in three anhydrous polymorphs – calcite, vaterite and aragonite. Although vaterite is the least thermodynamically stable polymorph, it attracts the most attention in various topics – drug delivery, tissue engineering or personal care application [1]. Vaterite has higher solubility in water than calcite and aragonite, therefore, vaterite crystalizes into calcite in water solution [2].

The knowledge of the conditions for controlled synthesis of vaterite microparticles plays the crucial role for further application. In this work, $CaCO_3$ microparticles were synthetized by precipitation from sodium carbonate and calcium chloride solutions in a special reactor with precise control of the temperature and rotation speed by thermal bath and mechanical stirrer. The effect of temperature and time on formation dynamic of $CaCO_3$ microparticles was investigated by the scanning electron microscopy (particles size and shape), fourier transformed infrared spectroscopy and X-ray powder diffraction was used to resolve vaterite and calcite ratio.

Figure 1 shows synthetized particles in temperature range from 10 to 50°C. Spherical shape was obtained for lower temperature, cauliflower and croissant shape for higher temperature and cubic shape for the highest temperature.

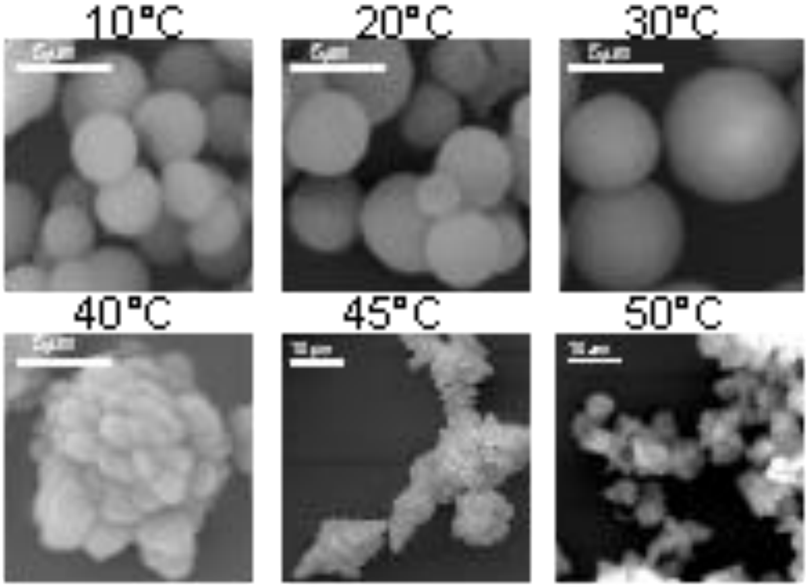

Figure 1: Obtained particles within the temperature range.

It was found out that both factors: reaction time and temperature affect particle shape and size significantly and allows to obtain the particles in size range from (3.5±0.8 μm till 19.8±5.8 μm). Moreover, longer reaction time favors crystallization of vaterite to calcite. Such type of particles possible to use in pharmaceutical area as drug delivery system.

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O19. The factors affecting the photocatalytic degradation of organic pollutants under visible irradiation using TiO_2/rGO nanocomposites as photocatalysts

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At the beginning of the 21st century, mankind has to face the problem of availability of water as an important threat, due to the loss of the balance between the quantity and quality of available water [1]. The ubiquitous organic pollutants (drugs, pesticides, and organic dyes) have become a matter of increasing concern. They have raised considerable concerns due to their frequent detection in drinking water, groundwater, and surface water, usually in the very low concentration [2]. Organic pollutants and also their metabolites can be toxic and some of them even carcinogenic for humans. Therefore, pollutants should be removed by an appropriate purification method. It was shown how various organic pollutants can be efficiently removed by photocatalytic processes in the presence of different catalysts. Heterogeneous photocatalysis with appropriate photocatalysts is among the most promising methods for the efficient removal of pollutants. It is a clean, green, sustainable and cheap method [1,2].

The nanocomposite photocatalyst based on titanium dioxide (TiO_2) and reduced graphene oxide (rGO) was produced. The material was prepared using a direct sol-gel method followed by hydrothermal treatment at different experimental conditions (e.g., pH, time, temperature) with the aim to optimize photocatalytic degradation.

Graphene oxide (GO) was produced from graphite flakes following a Hummer's method [3]. TiO_2 sol was prepared from titanium tetraisopropoxide as a precursor, *i*-propanol as a solvent, acetylacetone as a chelating agent and nitric acid as a catalyst [4]. TiO_2 nanoparticles and TiO_2/rGO nanocomposites, with different amounts of GO, were obtained by a hydrothermal method, where also time, temperature and pH of the treated suspensions were adjusted. The influence of the preparation conditions on the physico-chemical properties of synthesized powders was established by different characterization methods such as (powder X-ray diffraction analysis, Fourier transform infrared spectroscopy, scanning electron microscopy and Raman spectroscopy). Photocatalytic degradation of organic pollutants (caffeine, methylene blue) under visible light irradiation was used as a test reaction. The efficiency of the photocatalytic degradation was monitored by UV-Vis spectrophotometry.

Obtained results show how photocatalytic properties of prepared TiO_2 nanoparticles and TiO_2/rGO nanocomposites depend on different experimental parameters of their synthesis.

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O20. Spark plasma sintering of alumina ceramics with addition of waste alumina powder

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During industrial production of ceramic materials are observed process losses such as broken ware from shaping, drying, firing and refractory material, different kinds of sludge, dust, and used plaster molds. Some of the accumulated process losses mentioned above can be recycled and reused within the plant due to product specifications or process requirements; otherwise, remaining materials are considered as waste and are supplied to external recycling or disposal facilities. European Commission recently adopted an ambitious Circular Economy Action Plan, which proposes actions that should help to “close the loop” of a product lifecycle by reducing the generated waste, reusing the waste, and recycling where possible. The aim of this research was to investigate the possibility of recycling waste alumina powder. In this study, the high-purity alumina powder and waste alumina powder obtained after the green machining were used as raw materials. The powder mixture was suspended in ethanol and then subjected to the ball milling process. The resulting slurry was dried and densified by Spark Plasma Sintering according to Box-Behnken design in order to determine the optimal sintering regime based on the obtained densities of sintered samples. The corresponding response density of each sintered sample was measured in distilled water using Archimede’s principle. Then, the Response Surface Method was applied to find the optimal value of each factor to obtain maximum density.

After the determination of the optimal sintering regime, the sample prepared with commercial alumina powder was sintered at optimal conditions and compared to the alumina/waste alumina sample. Additionally, the morphology of the sintered samples was examined by Scanning Electron Microscopy (SEM). The polished samples were submitted to the hardness and fracture toughness measurement by the Vickers indentation method. According to obtained data the waste alumina powder could be used as secondary raw material to produce high quality advanced ceramics.

O21. A 1.6 V SOLID STATE SYMMETRICAL SUPERCAPACITOR USING NEEM LEAVES DERIVED ACTIVATED CARBON

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ABSTRACT

Bio-wastes are the great source of activated carbon possessing good electrical conductivity and high specific surface area. Herein, neem leaves derived activated carbon (NDAC) is synthesized which shows hierarchal pore size distribution along with good conductivity. Furthermore, the NDAC electrode shows superior electrochemical performance when tested in 1 M H_2SO_4 aqueous electrolyte. A high specific capacitance of 828 F/g is achieved even at a high current density of 2 A/g in three electrode system. Furthermore, an all-solid-state symmetrical supercapacitor is assembled using two equally weighted NDAC electrodes and PVA-1M H_2SO_4 polymer gel electrolyte within a potential window of 0-1.6 V. The NDAC//NDAC based solid state device delivers a high energy density of ~23 Wh/kg and a high-power density of 1.5 kW/kg along with a long cycle life of ~84% (after 5000 charge-discharge cycles). These results give the new directions for the application of low cost bio-wastes for next generation high energy density supercapacitors.

1. INTRODUCTION

Supercapacitors are the alternative energy storage devices having high specific capacitance, long cycle life, high power density but moderate energy density [1]. Therefore, it is always desirable to enhance the energy density of supercapacitors while employing novel electrode materials having high specific surface area and good conductivity. In this work, we have employed NDAC as an alternative active electrode material for supercapacitors possessing high porosity and good conductivity [2,3]. The NDAC based solid state supercapacitor shows promising results in terms of long cycle life, high energy and power density and thus becomes a superior electrode for next generation energy storage devices.

2. MATERIALS AND METHODOLOGY

Synthesis of NDAC

The NDAC is prepared through simple one pot hydrothermal pre-carbonization followed by KOH activation. Briefly, neem leaves are washed and dried in oven followed by grinding to form a fine powder. For pre-carbonization, the fine powder is immersed in 1 M H_2SO_4 in Teflon lined autoclave and heated at 180 ºC for 24 hours. After pre-carbonization, the obtained material is mixed with KOH in a ratio of 2:1 (KOH: material). After that the mixture is activated at 800 ºC for 3 hours in the presence of Argon atmosphere. Finally the obtained product is dissolved in 1 M HCl to remove the potassium content. Finally, the obtained material is centrifuged and washed with DI water and ethanol for several times and dried in oven at 80 C for 12 hours to obtain a final NDAC product.

3. RESULTS

The formation of NDAC is confirmed by XRD, Raman and FESEM characterizations. Figure 1 (a) shows Raman spectra of NDAC material in which the D and G bands confirms the formation of NDAC sheets. The broad peaks around 1369 cm^{-1} and 1592 cm^{-1} show the D and G bands respectively. Further, the electrochemical performance of NDAC electrode is tested using cyclic voltammetry (CV), galvanostatic charge discharge (GCD) and electrochemical impedance spectroscopy (EIS) techniques in 1 M H_2SO_4 aqueous electrolyte in three electrode system. Furthermore, an all solid-state symmetrical supercapacitor is assembled using two NDAC electrodes and PVA-1 M H_2SO_4 polymer gel electrolyte. Firstly, the device is optimized to obtain an operating potential window of 0-1.6 V. Using GCD analysis the device shows a high energy density of ~23 Wh/kg along with a high power density of 1.5 kW/kg (Figure 1(b)). Figure 1 (c) shows that the NDAC based solid state supercapacitor retain a long cyclic stability of ~84% after 5000 charge-discharge cycles.

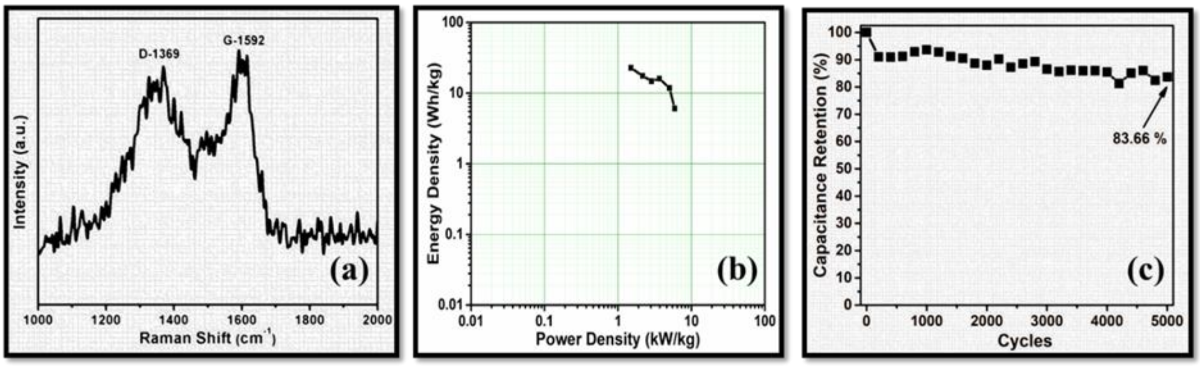

Figure 1. (a) Raman spectra of NDAC, (b) Ragone plot and (c) Cyclic stability plot for NDAC//NDAC solid-state symmetrical supercapacitor

4. CONCLUSION

In this work, neem leaves are used as bio-waste resource for the synthesis of highly porous and conductive activated carbon. Owing to these phenomenal characteristics, the NDAC material is used as an active electrode material for supercapacitor applications. The NDAC electrode shows very good electrochemical performance when tested in 1 M H_2SO_4 electrolyte in three electrode system. Inspired by these performance metrics, an all-solid-state 1.6V symmetrical supercapacitor is assembled and tested. The NDAC//NDAC supercapacitor shows an extraordinary cycle life of ~84% (after 5000 cycles) along with a high energy density of 23 Wh/kg. These results open a new path to use bio-wastes as an active electrode material for supercapacitors.

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O22. UiO-66 Derived Novel ZrO_2/C Composite For 2V ElectrochemicalCapacitor: An Approach to Conductive Additive Free Electrode Material

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ABSTRACT

Supercapacitors are gaining interest over other energy storage devices due to their high-power density, fast recharging and high cycle stability. However, designing an electrode material with high conductivity, mechanical robustness, and high surface area always remain a daunting challenge. Here in, we synthesize a novel zirconia nanoparticles (ZrO_2) and carbon composite from the pyrolysis of UiO-66 (a zirconium-based metal organic framework) with an approach to make it conductive additive free electrode material. The samples delivered the excellent specific capacitance of 241.5 F/g (at 1 A/g). Further, a symmetrical 2V solid state device (ZrO_2/C-1000//ZrO_2/C-1000) is assembled with PVA-1 M H_2SO_4 polymer gel electrolyte to determine its practical applicability. The assembled device delivers the high energy density of ~29 Wh/kg with a high-power density of 1.5 kW/kg and outstanding capacitance retention of 97 % after 2000 charging/discharging cycles. This outstanding electrochemical performance is attributed to the synergy between the ZrO_2 nanoparticles impregnated in conductive interconnected carbon skeleton having high surface area and meso-micro pores distribution.

1. INTRODUCTION

The downside and negative environmental impact of non-renewable source of energy had made the extensive commercialization of renewable sources of energy such as wind energy, solar energy etc(1). Supercapacitors or electrochemical capacitor are the excellent and unique energy storage devices due to its high-power density, long life and neutral impact over environment(2). Herein, we synthesize the zirconia nanoparticles confined in carbon skeleton (ZrO_2/C) by using the pyrolysis of UiO-66 (zirconium-based MOF) at different temperature to optimize the surface area of carbon and phase evolution of zirconia nanoparticles for supercapacitor.

2. MATERIALS AND METHODOLOGY

Zirconium chloride and BDC has been used for synthesis. The ZrO_2/C composites was prepared through the pyrolysis at different temperature of 600, 800 and 1000°C coded as Zr-600, Zr-800, and Zr-1000, respectively. For the preparation of the working electrode, the active ZrO_2/C composite material was mixed with polyvinylidene fluoride (PVDF) binder in a w/w ratio of 9:1 to form uniform slurry and then coated over a graffoil sheet.

3. RESULTS

The XRD pattern of the obtained ZrO_2/C composites (Fig 1a). All the peaks in the Zr-600 belongs to the cubic phase of the zirconium oxide(3). However, with the rise in temperature cubic phase changes to tetragonal phase. The Zr-800 sample exhibit the mixed cubic and monoclinic phase while Zr-1000 contain high percentage of monoclinic phase. To further confirm the presence of carbon, sample was characterized with Raman spectroscopy (Fig 1b). The broad peak around 1356 cm^{-1} and 1596 cm^{-1} corresponds to the D and G band respectively.

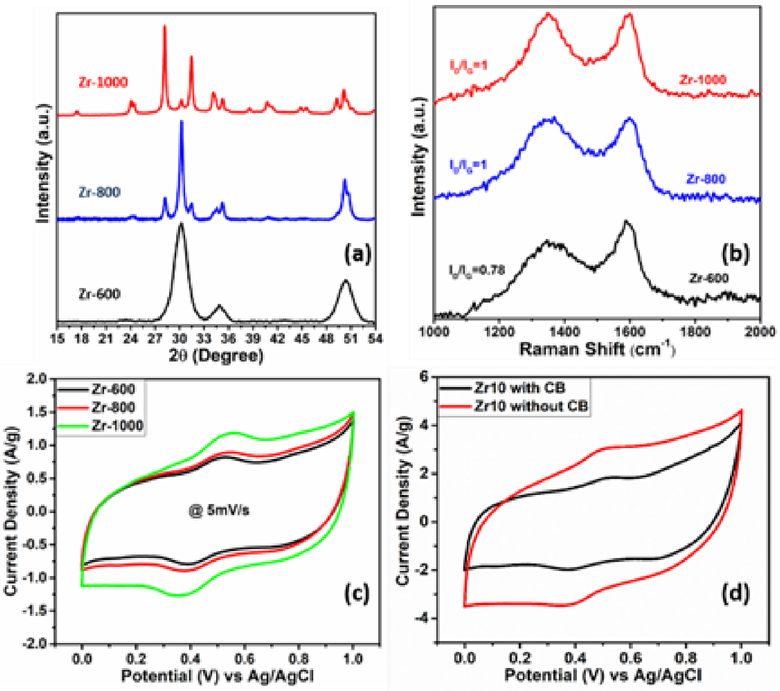

Figure 1 (a) XRD, (b) Raman spectra and (c) Cyclic Voltammetry of Zr-600, Zr-800, and Zr-1000; (d) Comparison of Zr-1000 with and without carbon black (CB).

The ZrO_2/C was further used to investigate the electrochemical performance through cyclic voltammery (CV) curve in 1 M H_2SO_4 (Fig 1c). The almost rectangular curve of CV demonstrates the fast ion transport and EDLC behaviour particularly due to the presence of carbon. The higher area of the CV curve of Zr-1000 demonstrates the higher specific capacitance. Additionally, the presence of small redox peaks demonstrates the redox activity of ZrO_2 nanoparticles in the pores of carbon. Further to demonstrate the conductive additive free approach another electrode with the addition of carbon black also tested with the CV curve. A comparison of both electrodes (Fig 1d). The higher area of the CV curve for conductive additive free electrode demonstrate the effective ZrO_2/C composites in which there is no need to add conductive additives to increase the conductivity.

4. CONCLUSION

The ZrO_2/C composites was synthesized from the pyrolysis of UiO-66 MOF at the different temperature. The sample Zr-1000 delivered the maximum specific capacitance of 241 F/g. When assembled as a full solid-state device with a gel electrolyte, the maximum energy density of 29 Wh/kg can be achieved at the high-power density of 1.5 kW/kg.

ACKNOWLEDGEMENT

Author would like to acknowledge the UGC and Director of CSIO for providing research grant, facilities and fellowship.

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O23. Tunable efficiency of Au-TiO$_2$ nanocomposites

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Au nanoparticles are commonly used nanomaterials for improving the sensing performance of surface plasmon resonance sensors. Surface plasmon resonance exhibit strong absorption corresponding to excitation wavelength regions. Consequently, a large electric field due to surface plasmon resonance is excited on the surface of the nanoparticles. The surface plasmon resonance sensitivity is closely related to the excited electric field. Therefore larger the electric field has more sensitive of surface plasmon resonance sensors to the change of its surrounding medium. This can help in increased stability and trapping capability of plasmonic nanoparticles that will boost the development of numerous applications in science and technology. The Au-TiO$_2$ nanocomposites show very interesting optical responses including nonlinear effects linked to absorption by surface plasmon resonance. The generated high energetic electrons in the plasmonic nanoparticles may migrate to TiO$_2$ surface if their energies are larger than the barrier at the interface between the Au and TiO$_2$. The energy of some electrons are not large enough surmount to barrier, they may also be injected into the TiO$_2$ oxide semiconductor through the tunneling effect. This can generate electron-hole pair, which can increase laser technology, organic pollutants, solar cell, sensor, photovoltaic and photo catalytic utilizations.

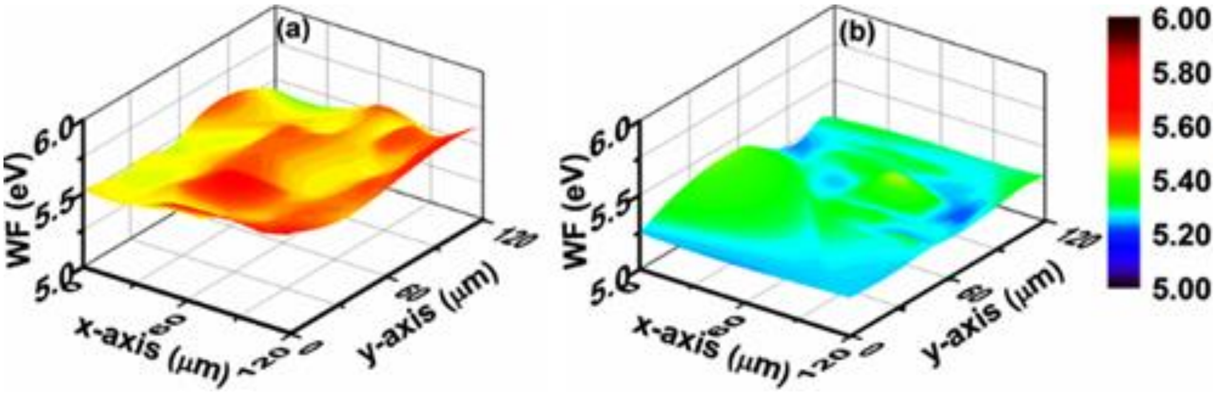

Figure: (a) Work function image of TiO$_2$ and (b) of Au-TiO$_2$ nanocomposite.

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O24. Novel hierarchical copper-based metal-organic frameworks for improved catalytic performance

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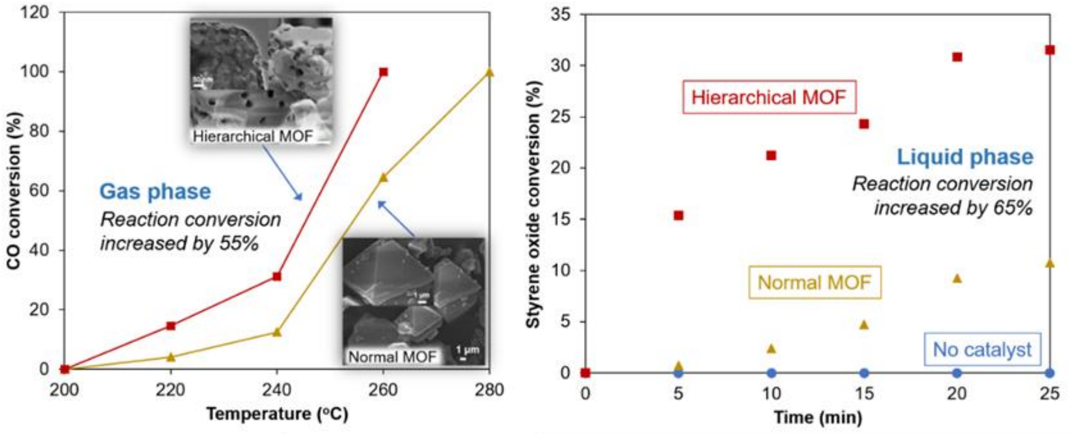
Introducing additional meso- or macroporosity into traditionally microporous metal-organic frameworks (MOFs) is a very promising way to improve the catalytic performance of these materials, mostly due to the resultant reductions of diffusional barriers during liquid-phase or gas-phase reactions. Here we show that HKUST-1 can be successfully synthesised either via post-synthetic treatment (etching prepared HKUST-1 samples in phosphoric acid) or via *in situ* crystallisation (exposing the MOF precursor solution to supercritical CO_2) to produce hierarchically porous structures that are highly beneficial for catalysis. These hierarchical MOFs were characterised by powder X-ray diffraction (PXRD), scanning electron microscopy (SEM) and gas sorption to confirm the preservation of the microscopic structure and the appearance of macropores in the crystallites. More importantly, the benefits of introducing these hierarchical porous structures into this MOF for improving the diffusion accessibility of reagents to the sample in catalysed liquid- and gas-phase reactions were quantified for the first time. It was found that the hierarchical pore structure helped to increase the reaction conversion of styrene oxide methanolysis (by ~65 % using either HKUST AE and HKUST CO_2, at 40 ^{o}C in 25 min) and CO oxidation (by ~55 % using HKUST CO_2 at 260 ^{o}C). These findings demonstrate the advantage of using hierarchical porous MOFs in catalysis.



a) b)

Figure 1. *Results of CO oxidative reactions (a) and styrene oxide methanolysis reactions (b), showing an improvement in activity for the hierarchical porous MOF (red), compared to normal microporous MOF (yellow)*

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O25. Electroactive materials based on polypyrrole coated electrospun nanofibers

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Actuator is a term which describes a device that transforms any kind of energy into mechanical motion. Such devices can find applications in various domains, the most appealing being biomedicine used as artificial muscles or organs [1], prostheses [2], outfits for rehabilitation and assistance [3], drug delivery and surgery devices etc. Introducing a sensing element into an actuator configuration will make the device to closely mimic the natural muscles, organ or limb. This work proposes a new actuator/sensor configuration fabricating using polymer nanofiber meshes obtained through electrospinning and conducting polymers. The electrospun nanofibers were covered with a thin metallic layer in order to electrochemically deposit polypyrrole (PPy) for making the nanofibers electroactive. The PPy coated networks were tested in actuator and sensor configuration. It was found that such material can act as mechanical sensor by sensing the modification of the load weight hanged on the sample. As well, the prepared material performs a movement during sensing process. All the measurements were registered by using an electrochemical cell, where the described material was used as working electrode, a platinum plate was used as counter electrode and Ag/AgCl as reference. The material was also morphological, structural and electrochemical characterized. The obtained results indicate that the fabricated fibrillary material can successfully be used in biomedical soft actuator development.

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O26. Characterization of sol-gel-derived ceria nanoparticles doped with manganese

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Ceria (CeO_2), with its stable fluorite structure and two interchangeable oxidation states, Ce^{4+} and Ce^{3+} has many excellent properties enabling its widespread use. Owing to the shift between Ce^{4+} and Ce^{3+}, oxygen vacancies occur within the lattice resulting with high oxygen mobility and oxygen storage capacity of ceria. Nanoparticles have a larger specific surface area compared to bulk material and thus provide faster oxygen exchange, resulting in better catalytic activity. It is belived that incorporation of Mn atoms in ceria crystal lattice will ensure even better catalytic propeties for oxidation of numerous compounds, for instance: carbon monoxide, phenol, and volatile organic compounds. With all this in mind, nano-ceria doped with manganese in various amounts was prepared via sol-gel synthesis. The as prepared samples were thermally treated to observe coarsening and thermal stability. All samples, as prepared and annealed, were studied by X-ray diffraction (XRD). Along with ceria, manganese (II) 2,4-pentadionate $[Mn(C_5H_7O_2)_2]$ lines appear in all of the as prepared samples doped with manganese. Crystallite size decrease due to incorporation of Mn atoms in the ceria crystal lattice was established via Scherrer method. The determination of surface properties as well as pore volume was acquired using Brunauer-Emmet-Teller (BET) N_2 gas adsorption-desorption isotherms. Scanning electron microscope (SEM) analysis gave insight into sample morphology showing ceria nanoparticles. Thermally induced changes were monitored via differential thermal analysis and thermo-gravimetric analysis (DTA/TGA) giving insight into the decomposition of leftover organic phase.

O27. Synthesis and characterization of copper doped ceria nanocatalyst

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Ceria (CeO_2) has been widely applied as a viable alternative to expensive noble metal catalysts. Its beneficial properties include low price, good poisoning resistance, and high catalytic activity due to the facile Ce^{4+} / Ce^{3+} redox reaction, high oxygen mobility and oxygen storage capacity within the crystal lattice. Modern day catalyst design is focused on the preparation of nanoscale catalysts, which possess significantly improved properties in comparison to bulk materials. Incorporation of metal ions, such as transition metals, into the ceria crystal lattice can further improve catalytic properties of the prepared nanocatalyst.[1] In this work, pure and 10, 20, 30 and 40 mol. % copper doped nanocrystalline ceria was prepared via hydrothermal method. Samples were analyzed by X-ray diffraction analysis (XRD), transmission electron microscopy (TEM), N_2 gas adsorption-desorption isotherms and energy dispersive X-ray spectroscopy (EDS). Catalytic activity of the prepared nanocatalysts was determined on the basis of toluene oxidation process. It was established that the addition of copper enhances the catalytic activity of nanocrystalline ceria.

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O28. Cellulose acetate/Iron oxide nanocomposite films: synthesis, characterization and RB5 removal

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Water pollution imposes a sustainable development of the society and the world economy. To remediate the wastewater pollution there have been employed a number of efficient methods such as adsorption, chemical and biological degradation, coagulation and membranes processes. The membrane separation based on polymeric materials is one of the most promising technologies for separation operations[1]. Pursuing our past work[2,3], it is our purpose to synthesize cellulose acetate (CA) films with hematite nanoparticles, α–Fe_2O_3 NPs by the phase inversion technique, and characterize them in terms of surface roughness, chemical composition, thermal stability, optical and magnetic properties, and surface wettability. The adsorptive efficiency of the nanocomposites to a reactive dye, hydrolysed reactive black 5 (RB5), was tested under specified conditions of pH, dye concentration, film dosage, contact time and temperature. The photocatalytic performance of the films for degrading the hydrolysed RB5 is underway and their recyclability will be tested.

SEM analysis of the composite films showed the typical asymmetric structure of the CA matrix with pores size higher than the pristine film. ATR-FTIR spectra presented typical CA bands with increasing intensity of the OH vibrational peaks. The thermal and optical properties were increased with the presence of the filler, and the magnetic behaviour was similar to that of a capacitor material. The composites showed higher surface wettability. Additionally, the adsorption properties of the films to the RB5 were better at a neutral pH and increased with the contact time and temperature, attaining a maximum value after a short time. UV–Vis absorbance analysis indicated the removal of RB5 which is ascribed to major adsorption of the RB5 molecules onto CA/α–Fe_2O_3.

In summary, the films were successfully prepared and the NPs showed a reinforcement of the matrix properties due to the physical interactions between the matrix and the NPs. Moreover, the adsorption properties were affected by the experimental factors, as expectable, and in line with the surface charge in the films and the charge of RB5.

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O29. Graphene Quantum Dot Modified Screen Printed Carbon Electrodes for Cortisol Sensing

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ABSTRACT

Graphene Quantum dots (GQDs) have been widely employed for biosensing applications because of its properties like conducting nature, luminescence and large surface area. Graphene Quantum dots were synthesized by directly pyrolyzing citric acid. The synthesized graphene quantum dots produced blue luminescence in UV light. GQDs displayed a broad absorption peak near 360nm and also exhibit an excitation-independent behaviour. To the GQDs modified screen-printed carbon-based electrode (SPCE), DNA-aptamer specific to cortisol was immobilised through Π-Π bonding and characterized electrochemically. On the immobilization of the aptamer, there was a decrease in the current which further increased on binding with the cortisol. A "signal on" sensor was developed with limit of detection of 0.3 pg/ml.

1. INTRODUCTION

Biosensors are the devices used to detect the concentration of the analytes. Biosensors consists of a biological component known as bio-receptor and a physical component known as transducer. Biosensors provide various advantages such as ease of use, fast and sensitive detection over traditional techniques used to detect cortisol. In this work, we have synthesized graphene quantum dots for the modification of the screen-printed carbon electrode. GQDs provide high surface area for the immobilization of the bio-receptor i.e. aptamer and conducting nature of the GQDs was explored for sensing application.

2. MATERIALS AND METHODOLOGY

Synthesis of GQDs

GQDs were synthesized by the pyrolysis of citric acid as discussed somewhere[1]. Briefly, 2 g of citric acid was first heated to 200 °C for 5 min which converted it in to a pale-yellow colour liquid and then continued thermal treatment for further 30 min produced an orange-colour liquid. The obtained orange colour solution was dropwise added in to a freshly prepared 100 ml of 10mg/ml solution of NaOH under stirring conditions. After neutralization to pH 7, water soluble graphene quantum dots were obtained.

Fabrication of electrochemical aptasensor

SPCE is modified using 10µl of synthesized GQDs. GQDs were drop casted on the working area of the electrode and dried at 70 ºC in vacuum oven for 1 hour. 10 µl of aptamer were drop casted on GQDs modified electrode and incubated at room temperature of 1 hour. Different concentrations of cortisol ranging from 0.1 pg/ml to 100ng/ml were used to detect cortisol.

3. RESULTS

The formation of GQDs is confirmed by UV, PL and FT-IR characterization. Figure 1(a and b) shows the UV and PL of the GQDs. In UV, GQDs exhibited a broad absorption peak near 360nm due to Π-Π* transition of aromatic sp2 domains which is not present in the UV spectrum of citric acid. When GQDs were excited from 320 to 400nm, the PL emission exhibited at wavelength 465nm with increase in the intensity of emission wavelength. Carbon-based nanomaterials exhibit excitation-independent emission behaviour because of their uniform size distribution[2]. Further, electrode modifications were characterized electrochemically. As GQDs are conducting in nature, there was an increase in the current as compared to the bare carbon electrode. While on the immobilization of aptamer, there was decrease in current due to the negative charge present on aptamers. Figure 1c shows the increase in the current with increase in the cortisol concentration ranging from 0.1pg/ml to 100ng/ml. A limit of detection of 0.3 pg/ml was obtained.

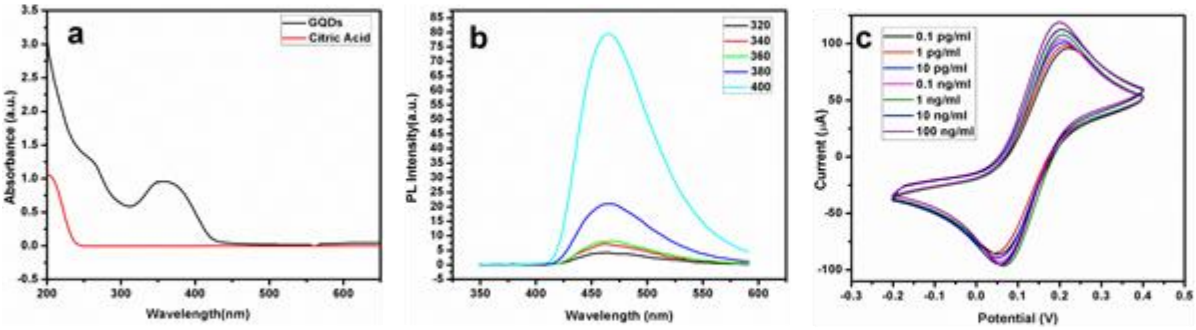

Figure 1 a) UV of GQDs and Citric Acid (b) PL of GQDs (c) CV plots of fabricated biosensor upon exposure to various concentration of cortisol

4. CONCLUSION

In this work, GQDs have been synthesized from citric acid and explored for the biosensing of the cortisol. Modification of GQDs SPCE with aptamers showed good results. Label free, signal on electrochemical sensor was developed to determine the detection limit and detection range. Sensor detected cortisol in a wide detection range of 0.1pg/ml to 100ng/ml with a very low detection limit of 0.3pg/ml.

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O30. Comparison between the performances of different boring bars in the internal turning of long overhangs

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Impact dampers are mainly used in the metal-mechanical industry in operations that generate too much vibration in the machining system. Internal turning processes become unstable during the machining of deep holes, in which the tool holder is used with long overhangs (high length-to-diameter ratios). The devices coupled to active dampers are expensive and require the use of advanced electronics. On the other hand, passive impact dampers (PID – Particle Impact Dampers) are cheaper alternatives that are easier to adapt to the machine's fixation system, once that in this last case a cavity filled with particles is simply added to the structure of the tool holder. The cavity dimensions and the diameter of the spheres are pre-determined. Thus, when passive dampers are employed during the machining process, the vibration is transferred from the tip of the tool to the structure of the boring bar, where it is absorbed by the fixation system. This work proposes to compare the behaviours of a conventional solid boring bar and of a boring bar with a passive impact damper in turning, while using the highest possible L/D (length-to-diameter ratio) of the tool and an Easy Fix fixation system (also called: Split Bushing Holding System). It is also intended to optimize the impact absorption parameters, as the filling percentage of the cavity and the diameter of the spheres. The test specimens were made of hardened material and machined in a CNC lathe. The laboratory tests showed that when the cavity of the boring bar is totally filled with minimally spaced spheres of the largest diameter, the gain in absorption allowed of obtaining, with an L/D equal to 6, the same surface roughness obtained when using the solid boring bar with an L/D equal to 3.4. The use of the passive particle impact damper resulted in, therefore, increased static stiffness and reduced deflexion of the tool.

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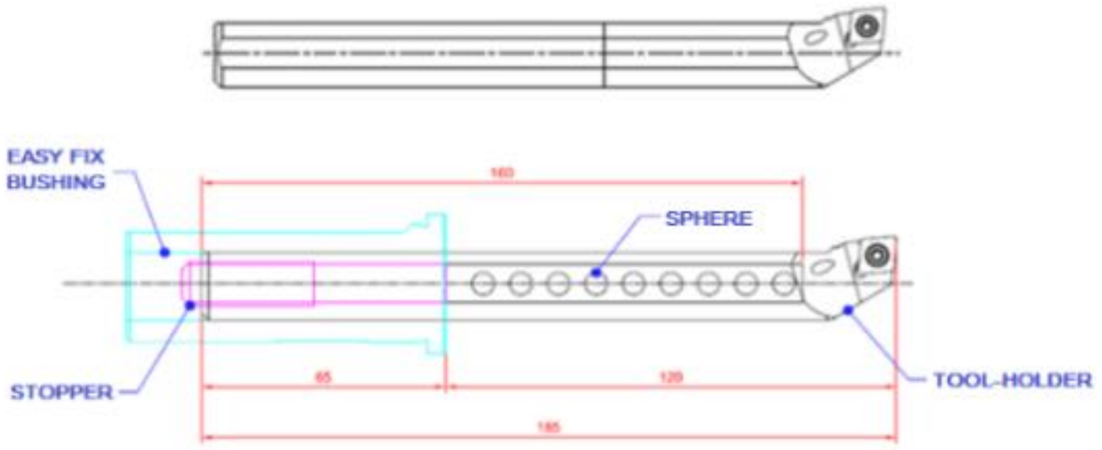

Fig. 1 Conventional boring bar (a) and boring bar with cavity (b)

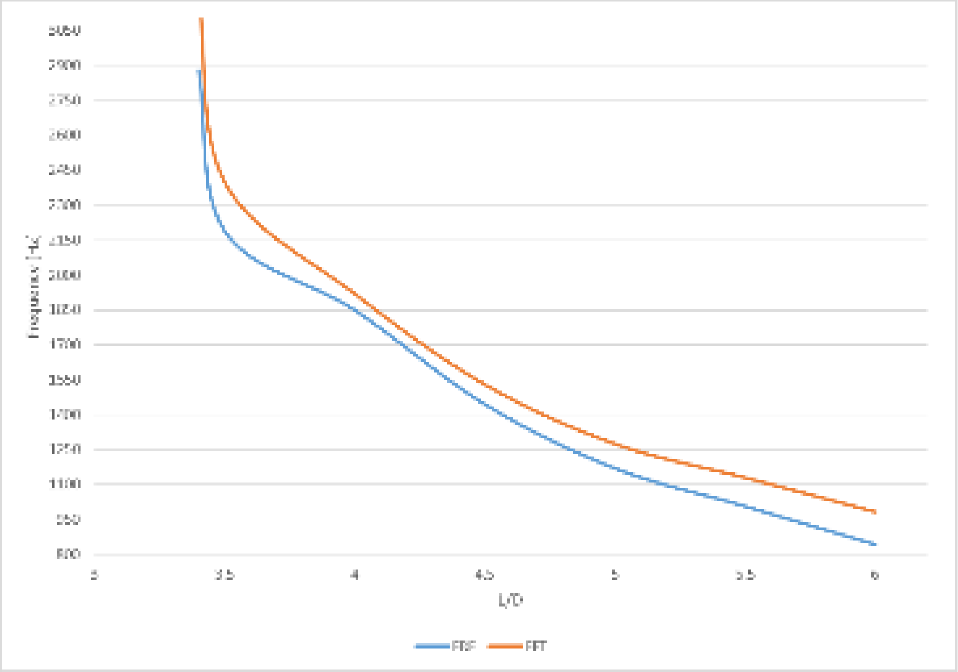

Fig. 2 Comparison between the FRF and the FFT of the boring bar with the best performance (boring bar filled with Ø 10,32 mm spheres).

O31. Mechanical properties of Twin Graphene Nanotubes: A molecular dynamics simulation

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One of the new nanotubes which recently take attention is twin Graphene nanotube (TGNT) to obtain new physical properties [1]. In this study, we used the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package [2] for investigating the mechanical properties of these nanotubes, which are formed by rolling up a twin Graphene sheet in a similar way with carbon nanotubes. TGNTs are include the carbon atoms in the sp and sp^2 hybridized states [3]. The adaptive intermolecular reactive empirical bond order (AIREBO) potential was used to describe the interactions among the bonded and The Lennard-Jones potential acted between the nonbonded atoms. Periodic boundary condition is applied along the nanotube axis, also the systems with different diameters were equilibrated in the canonical ensemble (NPT; constant number of atoms, temperature and pressure) during 1ns at 300K. After equilibration, the deformations of TGNTs under axial tension are conducted to obtain stress-strain diagram. Furthermore, the effect of TGNT diameter size, temperature and engineering stress rate on Young's modulus, fracture strength and strain of TGNTs are carried out.

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O32. Simulation of interacting and non-interacting dipolar systems and their temperature dependencies

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Dielectric systems are modeled to investigate relaxational phenomena for interacting and non-interacting cases. The systems are made up of randomly distributed dipoles in 3D space. The dipoles fluctuate due to thermal activation in double well potentials. The barrier height between the wells is assumed to be proportional to the distance between the wells. Two different systems, one with fixed dipole lengths having a single relaxation time and the other with distributed dipole lengths accounting for distributed relaxation times are investigated. A Monte-Carlo simulation technique, which involves the calculation of local fields at every dipole site using the method of images [1], is employed to compute iteratively the time dependent polarization.

As expected, a non-interacting system with distributed dipole lengths i.e. with a distribution of relaxation times exhibits a broadened response. However, it was found that the interaction between dipoles in systems with a single relaxation time also produces a broadened relaxational response. The interaction in systems with a distribution of relaxation times stretches the response further more. A field reversal experiment allows the discrimination between dipolar interaction and a distribution of relaxation times as a cause for a broadened response [2].

Also, these systems were further examined for the temperature dependence of the mean relaxation time τ. The temperature dependence revealed that the mean τ values exhibit for all interacting systems a Vogel-Fulcher behavior and for non-interacting systems an Arrhenius law.

Acknowledgements: The work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – KL 654/41-1.

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O33. Mesoscopic self-ordering in the (2×1) cerium-molybdenum(112) nanostructures

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Recently there is a growing interest in the properties of thin films and nanoparticles of rare-earth metals. In particular, nanoparticles containing cerium are found to be efficient in the treatment of dangerous diseases (see e.g. [1]). In this work, we have used Auger electron spectroscopy (AES), low-energy electron diffraction (LEED), contact potential difference measurements and density functional theory (DFT) calculations to study submonolayer adsorption of Ce on the molybdenum (112) surface. The growth of a monolayer film with a p(2×1) structure is observed at room temperature starting from the earliest stage of Ce deposition and up to adatom coverage of $\theta = 0.5$. Various low-coverage adsorbate structures have been examined by DFT calculations, showing the c(2×2) and p(2×1) structures to be energetically preferable. The work function Φ of the surface decreases with growing coverage and $\Delta\Phi$ reaches a minimum value of –2.2 eV at $\theta = 0.5$. The film deposited at room temperature is poorly ordered, but the order degree is enhanced under annealing at gradually increasing temperatures in the range of T_a = 300−1500 K. As evidenced by the AES data, exceeding this temperature range causes partial desorption of Ce. The p(2×1) order degree attained under annealing depends on the coverage. To estimate the order degree, we have used the full halfwidth values $\Delta_{(2\times1)}$ of the LEED beams' intensity. High order degree is registered for $\theta \approx 0.5$: annealing up to 800−1000 K provides the $\Delta_{(2\times1)} \approx 3$ % of the surface Brillouin zone (SBZ) size, which is close to the coherence width of our LEED device. Below $\theta \approx 0.5$ the p(2×1) order obtained as a result of annealing up to 1500 K is poorer the lower the coverage. In a broad coverage range $\theta = 0.1−0.45$, annealing at $T_a \geq 1200$ K creates a p(n×1) LEED pattern which coexists with that of the p(2×1). The p(n×1) features appear as satellites split from the integral-order spots by SBZ/n units along the [111] direction. At $\theta \approx 0.1$ we observe $n = 23$, which corresponds to the formation of p(2×1) domains with a long-range (mesoscopic) 1D periodicity of 23 substrate units (about 63 Å). With coverage growing to $\theta \approx 0.25$, the observed value of n increases a little (up to 26), but at $\theta > 0.35$ the splitting spots approach the integral-order spots and become unresolved. In conclusion, the formation of a 1D mesoscopic domain p(2×1)Ce/Mo(112) structure has been detected which is discussed in terms of surface stress driving force.

O34. CFRP Use in SLV Propellant Tanks - Concept and FEM Study

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Weight reduction is a never-ending objective in aerospace engineering, particularly, for a space launch vehicle (SLV) were every gram of mass has a penalty in the vehicle's performance. With the propellant tanks generally having more than half of a SLV's dry mass [1], it is straight forward that composite materials should be implemented in their construction. However, difficulties with oxygen compatibility, permeability and fabrication maturation dictate that Aluminum alloys with high Lithium content are still the state of the art in this field [2]. Recent developments and a maturation of the aerospace composites industry are starting to change this perception, particularly, regarding carbon fiber reinforced polymer (CFRP) application [3]. Hence, this study aims to propose an integral CFRP propellant tank concept and determine mass savings by comparing it to a metallic baseline, through finite element method (FEM) analysis with simulated flight loads. Tank dimensions, geometry and loads were chosen for micro-satellite SLV application. Also, Altair's Optistruct solver was used for FEM calculations, with Altair's HyperWorks for pre and post-processing. A mass reduction of close to 35% has been achieved with comparison to the metallic baseline design for same boundary conditions. Therefore a sound and competitive design for a micro-satellite SLV propellant tank has been achieved.

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O35. Whole-particle models of atomic arrangements in brookite titania nanorods

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Promising photocatalytic properties have been reported for nanoparticles of all three common TiO_2 polymorphs and mixtures thereof. The superior performance of the brookite nanorods has been attributed to slower electron-hole recombination after the absorption of light. Yet, the mechanism responsible for this effect remains unclear. In nanoparticles, structural relaxations induced by the finite size and free surfaces are expected to modify the electronic structure relative to the bulk prototypes. However, the exact structure-property relations remain uncertain in part because such distortions themselves have not yet been characterized in detail.

Traditional crystallographic techniques that assume periodic atomic order become ineffective when applied to intrinsically aperiodic nanocrystals. Little is known about atomic relaxations in these materials relative to bulk crystals.

Over the last two decades, alternative techniques have been developed to address this so-called “nanostructure problem”. These methods utilize X-ray/neutron total scattering which is related to instantaneous interatomic distances via the Debye formula. This relationship can be used either to fit a structural model to a total-scattering signal directly in reciprocal space or to transform total-scattering data into real space to yield an atomic pair-distribution function, which is then fitted to determine structural characteristics. The basic models employ an asymmetric unit and space-group symmetry, analogous to descriptions of bulk crystals. The resulting nanoparticle structure is then refined against experimental data, with structural variables typically limited to lattice parameters, coordinates of symmetrically inequivalent atomic positions, and atomic displacement parameters. While providing an overall assessment of structural order, symmetry-constrained models cannot resolve structural relaxations at particle surfaces or identify spatially variable distortions.

An alternative approach involves using an atomistic configuration that represents a snapshot of a whole-nanoparticle structure. Typically, these types of refinements are performed using a Reverse Monte Carlo (RMC) method.

Structural refinements of whole-nanoparticle atomistic models using X-ray total-scattering data and the RMC algorithm were demonstrated for mixtures of TiO_2 brookite nanorods and irregularly shaped anatase nanoparticles. The brookite and anatase nanocrystals were shown to undergo lattice-volume expansion and contraction relative to their bulk prototypes. The atomic positions in the nanorods differed from the bulk structure by an effective shift of the Ti Wyckoff position in the brookite unit cell, combined with additional static atomic displacements that increased progressively from the nanorod axis toward its side surfaces.

The soundness of the obtained characteristics was assessed using first principles calculations, which produced the results that were in qualitative agreement with the experimental observations and additionally revealed a strong dependence of the structural relaxations, including lattice-volume changes, on sorbate coverage.

O36. Oxide thermoelectrics prepared by laser melting: effects of processing atmosphere

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Thermoelectric materials can convert waste heat into electrical energy, thus contributing to the sustainable energy technologies. Traditional thermoelectric materials, despite their good performance, suffer from two main problems, the toxicity/scarcity of the elements used and their stability in harsher work conditions like high temperatures or non-inert atmospheres. Thermoelectric oxides appear to be a promising alternative due to natural abundance of the constituents and high thermal stability [1]. This work focus on the processing of these materials using the Laser Floating Zone (LFZ) technique, with particular emphasis given to laser processing under various redox atmospheres, allowing unique opportunities for tuning the structural, microstructural and thermoelectric properties [2], including growth of fully dense fibres, formation of metastable phases and/or promoting different oxidation states by adjusting the growth conditions. Here we report the processing of model manganite- and titanate-based materials including donor-substituted Ca(Pr)MnO$_3$ and Ti(Ta)O$_2$ systems. The results suggest successful incorporation of the dopants in the structures of the base material. Electrical conductivity studies and microstructural characterization of the Ca(Pr)MnO$_3$ samples indicate the formation of core-shell structures with different resistivities. These core-shell structures are not always desirable and may negatively affect the transport properties, as observed when compared to the Ti(Ta)O$_2$ system. This work shows how these structures can be tuned or eliminated by a posterior thermal treatment. XRD/SEM/EDS studies demonstrate some guidelines for tuning the phase composition and microstructure by adjusting the growth rate under different redox conditions. We report high power factor values of 303 $\mu Wm^{-1}K^{-2}$ at 1120 K for the Ca(Pr)MnO$_3$ system [3] and 317 $\mu Wm^{-1}K^{-2}$ for the Ti(Ta)O$_2$ system. The obtained guidelines suggest that LFZ is a suitable technique for processing thermoelectric oxides, if optimized control over growth parameters and re-equilibration conditions is imposed.

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O37. Electrical performance tuning in thermoelectric $Ca_3Co_4O_9$ materials by transition metals additions

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This work reports on the effects on high-temperature thermoelectric (TE) properties in bulk, polycrystalline p-type $Ca_3Co_4O_9$ ceramics, after employing a composite approach consisting of metallic particles additions and two simple sintering schemes. The added Fe, Co and Ni particles are expected to act as porosity fillers upon oxidation in air and provide improved grain connectivity, changing the microstructural features and electrical properties of the resulted materials. The composites have been prepared through a modified Pechini method, followed by one- and two-stage sintering, to produce low-density (one-stage, 1ST) and high-density (two-stage, 2ST) ceramic samples. The electrical conductivity (σ), Seebeck coeffcient (α) and power factor (PF) values have been investigated between 475 and 975 K, in air flow, and related to the sample's respective phase compositions, morphologies and microstructures. For the Co additions in the 1ST sintering case, the porous samples reached maximum PF values of around 210 $\mu Wm^{-1}K^{-2}$, being around two times higher than those of the pure $Ca_3Co_4O_9$ matrix. For the 1ST-sintered Fe and Ni added samples, the highest PF values of 80 and 90 $\mu Wm^{-1}K^{-2}$ have been measured for the 3% vol. Ni and 3 and 6% vol. Fe additions, respectively, very close to some of the best reported values from literature. In contrast, 2ST sintering resulted in much denser samples and more complex phase compositions and microstructures, leading to lower electrical performance. The improvements of electrical properties achieved in the present work are promoted by a simultaneous increase in electrical conductivity and Seebeck coefficient values, stemming from pore filling effects and subsequent microstructural modifications.

O38. ZnO-modified BZY upon different B-site locations

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Three different mechanisms for addition of 4 mol% ZnO sintering additive to the leading proton-conducting perovskite Ba(Zr,Y)$O_{3-\delta}$ (BZY) involving substitution for Y, Zr or B-cation excess have been analysed in terms of densification, dopant location, microstructure and electrical properties. Our results reveal that the addition of ZnO to the BZY phase promotes high levels of densification (up to 98% of the theoretical value) at 1300 °C, irrespective of initial stoichiometry. Analysis by scanning transmission electron microscopy-energy dispersive X-ray spectroscopy indicates that Zn resides in both grains and grain boundaries for all Zn-containing stoichiometries, with a greater grain-boundary concentration observed for a B-site excess mechanism. The concentration of ZnO in the intergranular regions is proportional to both the degree of inhibition of grain growth and enhancement of the dominant low-temperature specific grain-boundary conductivity. Partial conductivities determination demonstrates that the addition of ZnO in substitution for the Zr site provides the highest values of bulk protonic conductivity due to the higher hydration enthalpy. In contrast, the B-site excess mechanism provides higher specific grain boundary conductivity, as a result of the lower depletion of charge carrier in the grain boundary space-charge layers. This work explains for the first time that the way the sintering additive is included in the perovskite phase leads to important differences in the transport properties of the densified resultant proton-conducting ceramic, providing new insights in the development of future processing routes for the application of these materials.

Acknowledgements

The authors also acknowledge the projects POCI-01-0145-FEDER-032241, UID/EMS/00481/2019-FCT – FCT - Fundação para a Ciência e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF).

O39. The influence of ammonolysis temperature on physical properties of vanadium oxynitride (VO_xN_{1-x}) solid solutions

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Transition metal nitrides are attractive materials due to their notable catalytic and electronic properties [1]. In particular, vanadium (oxy)nitrides have generated high interest due to their wide applicability in heterogenous catalysis [1], energy related research (e.g. supercapacitors) [2] and also superconductors [3]. Their suitability for these applications strongly depends on the N/O ratio in their structure. Hence, in this work, several oxynitrides, (VO_xN_{1-x}, $0 < x < 1$), are prepared by the ammonolysis route, by conversion of the parent oxides under flowing gaseous ammonia at high temperatures, to establish correlations between the synthesis temperature and the resultant structural, chemical and optical properties. Powders are characterized by combining X-ray powder diffraction (XRD), thermogravimetry (TGA), X-ray photoelectron spectroscopy (XPS), and diffuse reflectance spectroscopy (DRS) This work highlights the possibility to precisely control chemical composition and N/O ratio by ammonolysis temperature, thereby providing an exciting new method for materials tailoring.

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O40. Proteic sol-gel synthesis of Gd-doped ceria electrolytes

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We propose an innovative, cheap and environmentally friendly route known as “proteic sol-gel synthesis” using commercial flavorless gelatin as polymerizing agent [1] to prepare Gd-doped ceria materials ($Ce_{1-x}Gd_xO_{2-\delta}$, x = 0, 0.1 and 0.2), a common electrolyte material in Solid Oxide Fuel Cells. Materials were comprehensively characterized for their structural, microstructural, and electrical properties using several techniques. The results reveal the high competitiveness of the proposed synthesis route, where dense CGO electrolytes can be obtained at the sintering temperature 1350 °C, a significantly lower temperature than the majority of standard processes. Results show improved bulk conductivity in the composition containing 10 mol% Gd, while no significant differences exist in the specific grain boundary properties. This work provides a novel route for the synthesis of CGO ceramics with competitive performance and decreased sintering temperature.

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Acknowledgements

The authors acknowledge Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq/Brazil, reference number 200439/2019-7) and the projects POCI-01-0145-FEDER-032241, UID/EMS/00481/2019-FCT and CENTRO-01-0145-FEDER-022083 – funded by FEDER, Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF) and by national funds (OE), through FCT/MCTES.

O41. Niobium nitride as electrocatalyst for ammonia synthesis: synthesis and stability conditions

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A principal aim of the Horizon 2020 program is reduction in carbon dioxide emissions by the development of new technological methods for industries and their processes. Interest in ammonia (NH_3) synthesis research has been increasing over the past years due to its application in many essential products such as medicines and fertilizers. 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 alternative fabrication technologies, where one of the most promising is the direct electrochemical synthesis of NH_3 from steam and nitrogen [4].

One of the limitations of the process is the competition of the hydrogen evolution reaction with the ammonia synthesis reaction on the cathodic electrode [1,5]. Therefore, the search for a catalyst that can offer suitable catalytic properties is essential. Transition metal nitrides have been highlighted by DFT calculations to offer high catalytic activity for the ammonia formation reaction, whilst suppressing H_2 evolution (HER) [6,7] .

In this work, we preliminary study on the synthesis and stability of niobium nitride as a potential electrocatalyst for ammonia synthesis.

Acknowledgements

The authors acknowledge the projects SFRH/BD/130218/2017; POCI-01-0145-FEDER-032241, UID/EMS/00481/2019-FCT and CENTRO-01-0145-FEDER-022083 – funded by FEDER, Centro Portugal Regional Operational Programme (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF) and by national funds (OE), through FCT/MCTES.

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O42. Interfacial Integrity Enhancement of Atomic Layer Deposited Alumina on Boron Doped Diamond by Surface Plasma Functionalization

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High dielectric constant (high-κ) thin films are ubiquitous in research as they impart enhanced properties to microelectronic applications[1,2]. Novel combinations for coupling high-κ and ultra-wide band gap semiconductors are being investigated for niche applications, dependent on the environmental conditions for device operation[3]. Typically, high-κ films such as alumina are deposited by atomic layer deposition (ALD), a technique heavily dependent on surface chemistry. This work investigates the effect of plasma surface functionalization of boron doped diamond (BDD) semiconducting films on interface quality with top-layers of ALD alumina (AlO) films, by analyzing its susceptibility to deformation; being particularly vital for electronics subjected to physically demanding environments. Alumina thin films were deposited unto as-grown (AlO-H-BDD) and O_2 plasma treated (AlO-O-BDD) polycrystalline BDD. XPS analysis performed on plasma exposed BDD films, prior to AlO deposition, demonstrated a 3% increase in O surface ligands compared to the as-grown surface. Nanoindentation analysis demonstrated plastic deformation within the alumina layer for AlO-O-BDD, for the tested loads, whereas AlO-H-BDD experienced film delamination and deformation beyond the alumina-BDD interface. TEM analysis revealed that delamination was most likely due to low cohesive strength of alumina near the interface, explained by fewer –OH and –CO (ether) BDD surface ligands on H-BDD.

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O43. Cobalt decorated TiO_2 nanosheet as high pseudocapacitance cathode for long lasting rechargeable Mg-Li hybrid batteries

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Magnesium batteries in recent years have proposed and investigated as one of the apt post lithium batteries because of its large theoretical volumetric capacity (3833mAh/cm^3), natural abundance (2.7%) low material cost (~$2000/ton) and dendrite free redox reactions[1]. However, due to the sluggish ion diffusion kinetics caused by the electrostatic hindrance from the host electrode's positive charges cloud, specific capacities of Mg batteries are limited[2]. Mg-Li hybrid batteries are a promising adaptation to bypass these drawbacks of these setbacks and to fully exploit its cost-effectiveness and safety advantages[3]. However, developing a dual ion compatible high-performance cathode is the practical hurdles of this hybrid battery system.

Herein, we present a high-rate and longlasting Mg-Li hybrid battery composed of metallic Mg anode, cobalt decorated TiO_2 nanosheet as the cathode and 0.4M APC (all phenyl complex) + 0.75M LiCl / THF electrolyte solution.

Optimized cobalt loading (8%) on the TiO_2 nanosheet, provided splendid electrochemical performance. Nano grain boundaries created at the TiO_2 and Co_3O_4 crystallites provided very large pseudocapacitive (up to 93%) characteristics. Hybrid nanosheet cathode also demonstrated excellent specific capacities (328 mAh/g at 25 mA/g) and rate performance (198 mAh/g at 1A/g). Further, it showed cycling stability of up to 3000 cycles at 1A/g current density with ~87% capacity retention and ~100% coulombic efficiency. The specific electrode designs imparting good structural stability is also contributed to the electrochemical characteristics during the charge-discharge process.

Exceptional electrochemical characteristics of Co_3O_4-TiO_2 hybrid nanosheet cathode is a result of the predominant pseudocapacitive type Mg/Li storage felicitated by superior diffusion of ions through nanointerfaces. Two-dimensional morphology, mesoporosity, high surface area and ultrathin nature are also contributed as secondary factors. The demonstrated methodology of nanointerfaces driven pseudocapacitance can be further extended for the development of numerous high performing electrodes for next-generation Mg-Li hybrid batteries.

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O44. Piezoresponse force microscopy of organic materials

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

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

This work is supported by the Portuguese Foundation for Science and Technology (FCT): IF/00582/2015, BI (DOUTOR)/6323/2018), UID/EMS/00481/2019-FCT and CENTRO-01-0145-FEDER-022083.

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Poster presentations

P1. Synthesis and characterization of green nanocomposites based on N-carbazole

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Green chemistry applies as well to the preparation of new products or more ecological processes as to the search for alternative solutions[1]. As part of this work, we sought to develop and characterize a synthesis of new classes of monomers, polymers and conductive nanocomposites based carbazole. The substitution of N-carbazole by epoxide group was obtained in two different ways, under microwave irradiation and conventional processes.

These monomers, polymers and nanocomposites are characterized and confirmed by infrared spectroscopy (FTIR), 1H and 13C nuclear magnetic resonance, Thermogravimetric Analysis (TGA).

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P2. The impact of β-myrcene and α - humulene on the lipid monolayers and bilayers imitating the plant pathogen bacteria membranes

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The essential oils have a wide range of biological activities. In this context it can be mentioned about antibacterial, antivirus, antifungal properties of these substances. In some cases they exhibit also the anticancer effect [1]. All of this makes the essential oils useful in medicine and pharmaceutical industry. The mentioned above properties could also be useful in the preparation of ecological pesticides based on the plant extracts. They could be a good alternative for the synthetic compound. From the latter point of view, the hop essential oil is very interesting and promising agent. As it was evidenced recently [2] β - myrcene and α - humulene are two main components of this essential oil. In fact, there is very little information in literature on the role of these two terpenes in antibacterial effect of the hop essential oil. On the other hand, before the commercial anti - pests use, it is necessary to identify and select the active compounds from the mixture, then to study on biochemical and molecular origin of its activity, and finally to evaluate its effectivity at various external conditions, safety dose and the most effective delivery formulation. The aim of this work was to compare the effect of myrcene and humulene on the lipid monolayers and bilayers imitating plant pathogen membranes. The experiments involved the surface pressure-area measurements, the penetration studies and Brewster angle microscopy experiments, as well as dynamic light scattering (DLS), zeta potential measurements and steady-state fluorescence anisotropy of DPH measurements. In results, it was found that both of the studied compounds modify the condensation and morphology of the lipid monolayers and alter permeability of liposomes. However, their effect is determined by their concentration and the membrane composition. The most important finding was that myrcene and humulene act on model membrane systems according to different mechanisms.

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P3. Interaction of polychlorinated biphenyls and chlorobenzoic acids with bacterial model membrane

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Polychlorinated biphenyls (PCBs) were extensively used as: oil in transformers, hydraulic fluids, adhesives, plasticizers, and pesticide extenders[1]. Due to their toxic and bioaccumulative potential, long range transport and persistence in the natural environment, PCBs were banned form usage and production[2]. However they still pose as an environmental threat. In fact, lower-chlorinated PCBs, such as PCB11 have been discovered to be byproducts of pigment production[3].

Due to hydrophobic nature, PCBs tend to adsorb onto particulate matter and soil organic matter and accumulate mainly in soil and sediments[1]. Natural soil and aquatic biota can come in contact with PCBs, and for the biodegradation process to occur it is of crucial importance PCB-biological membrane interaction. The main objective of this study was to investigate the interaction between PCBs with model biological membranes of soil decomposers.

The disubstituted PCBs investigated in this study were: PCB4, PCB11 and PCB15. Additionally water soluble metabolites were analyzed: 3,4-dichlorobenzoic acid, 2,5-dichlorobenzoic acid and 2,4,6-trichlorobenzoic acid. The mechanical properties of mixed monolayers were evaluated by surface pressure (π) – mean molecular area (A) isotherms registration. The observation of the film textures was accomplished through Brewster Angle Microscopy, while at a molecular level the structure was monitored by Grazing Incidence X-ray Diffraction (GIXD). As for the water soluble metabolites the penetration tests were performed.

The results suggest that the interactions between PCBs and phospholipids depend on the chlorine substitution, and in particular with the positions of the chlorine atoms: ortho-, meta-, para-. The better understanding of the PCB behavior towards the bacteria membrane could lead to a satisfactory usage of these organisms for the complete biodegradation of PCBs.

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P4. Synthesis of porous materials from fly ash

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Currently, fly ash from coal combustion is mainly used in cement production or as an additive in concrete, ceramics, and lightweight aggregates. Constantly tightening regulations regarding exhaust emissions from stationary sources force the use of various methods to reduce the emissions. This leads to the changes in mineral and chemical composition of the resulting fly ash which often prevents their use in the abovementioned applications. That is why new directions of using this waste should be sought.

The purpose of this work is to present the fly ash utilization to obtain materials with a developed specific surface area and a strictly defined pore structure allowing for wide application in environmental engineering. Three types of materials were obtained during the fly ash conversion reactions: (i) zeolites (Na-X, Na-P1, Na-A, ZSM-5), (ii) mesoporous silica materials (MCM-41, SBA-15), (iii) metal-organic frameworks (Al-MOF).

Structural characterization was made using X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The textual parameters were determined using nitrogen adsorption/desorption isotherms at liquid nitrogen temperature.

The results showed the ordered structural structure of all obtained materials and their monomineral character. The content of individual phases in the obtained materials was 98-100%. Analysis of textural parameters revealed microporous nature of Na-X and Na-A zeolites (the share of micropores was 71.2 and 71.8%, respectively). In contrast, zeolite Na-P1 and silica materials MCM-41 and SBA-15 and Al-MOF have a mesoporous character. The highest specific S_{BET} surface area was recorded for MCM-41 (1100 m^2/g) and the lowest for Na-A (71 m^2/g).

The materials obtained due to their high purity, relatively low cost of acquisition and physicochemical properties can be used to produce sorbents for removing impurities from water, sewage and gases. In addition, it is possible to modify their features relatively easily at the synthesis stage to obtain catalysts and photocatalysts.

The research was carried out as part of the TEAM-NET project - POIR.04.04.00-00-14E6/18-00 financed by Foundation for Polish Science

P5. The use of waste materials as ecological fillers in mix asphalt

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The construction of road surfaces is associated with significant consumption of natural resources including mineral aggregates and crude oil. In addition to mineral aggregates the filler is one of the major components of the asphalt mixture, which constitutes from a few to several percents. The limestone is acquired from natural mining deposits, which are constantly diminishing. Alternatively, waste materials can be applied as fillers in mix asphalt.

Two different fly ashes were used in the study as an alternative fillers/as filler additive: class F (FA-F) and class C(FA-C). These ashes were added to the mix asphalt (AC 11 S) together with lime filler in the lime/ash proportions of 3: 1, 1: 1, 1: 3. In total, tests were carried out for 7 types of asphalt mix.

Fillers **(**limestone and fly ashes) were characterized in terms of chemical composition (XRD), mineralogy (ED-XRF) and grain size (laser diffraction method).The following tests were performed on mix asphalt samples: maximum density (EN 12697-5), bulk density (EN 12697-6), air voids content (EN 12697-8) and water and frost resistance tests (EN 12697-12). The main results obtained are presented in Tables 1 and 2.

Table 1. Main chemical components of fly ashes [%]

	Na_2O	MgO	Al_2O_3	SiO_2	P_2O_5	SO_3	K_2O	CaO	TiO_2	Fe_2O_3	LOI
FA-C	0	1.039	14.69	43.97	0.118	6.89	0.164	22.12	1.885	6.726	2.4
FA-F	1.012	1.854	23.88	51.98	0.283	0.753	2.554	3.419	1.255	10.42	2.6

Table 2. Indirect tensile strength and water and frost resistance of mix asphalt AC 11 S

	AC	AC-F 3:1	AC-F 1:1	AC-F 1:3	AC-C 3:1	AC-C 1:1	AC-C 1:3
V_m [%]	1.2	1.2	1.4	1.6	1.3	1.9	2.8
ITSR [%]	93	96	103	104	103	104	102

Replacement of a part of the filler with fly ash has positively influenced the resistance to water and frost of the mix asphalt expressed by the ITSR index. For the samples with FA-F addition, the ITSR index was in the range of 96-104% whereas for the samples with FA-C addition it was 102-104%. An interesting result is the fact that even the samples with high air voids content (AC-C1: 3) had a high resistance to water and frost.The results indicate that both classes of fly ash can be applied to the mix asphalt as alternative mineral filler, since the air voids as well as resistance to water and frost of the obtained mix asphalt met the standards.

Funding: This research was financed within the statutory funds No. FN12/ILT/2019.

P6. Copolymerization of Maleic anhydride catalyzed by maghnite-H +

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Maghnite is a montmorillonite sheet silicate clay that is exchanged with protons to produce Maghnite-H+(Mag-H+). This non-toxic and cheaper cationic catalyst was used for the copolymerization of Maleic Anhydride (MA) with vinyl Acetate (VA). The effects of the amounts of Mag-H+, the temperature on the synthesis of poly (Maleic anhydrid-co-vinyl acetate) were studied.
The copolymer obtained was characterized by ^{1}H-NMR and IR spectroscopy, DSC, ATG.

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P7. Mesoporous material Si-MCM-41 synthesized from local kaolin DD1 as potential adsorbent for the removal of Hol Colex dye

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Two types of mesoporous Si-MCM-41 materials were synthesized via a cationic surfactant template method using raw and treated DD1 Kaolin. The mesoporous materials obtained were characterized by FTIR, XRD, BET, TEM techniques. However, DD1 Kaolin was used as Si precursor, a mesoporous Si-MCM-41 solid with hexagonal arranges and a long-range ordered structure could be obtained.

The adsorption tests were done using the "**Hol Colex**", commonly used in the paint industry. The results show that the adsorption is efficient and feasible at ambient temperature on DD1 kaolin issued mesoporous materials synthesised by DD1 kaolin with good discoloration efficiency. These experiments were carried out to determine the ideal conditions of pH, adsorbent mass, and contact time for the process. Adsorption isotherms, thermodynamic studies, and the treatment of cationic dye was also investigated.

P8. The structure of non-IPR isomer 28324 (C_1) of fullerene C_{80}

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Nearly 100 of non-IPR higher fullerenes have been produced last two decades as endohedral or exohedral derivatives [1]. All of them are synthesized by chance i.e. at start no one has known what would appear on finish. One of the reasons of such an uncertainty is very limited knowledge of molecular structure of pristine non-IPR fullerene. C_{80} fullerene has 31 924 cage isomers, but among them only seven satisfy the isolated pentagon rule (IPR). All non-IPR fullerenes are well-known to be unstable as pristine ones. Recently non-IPR fullerene C_{80} have been obtained in the electric-arc synthesis as actinide endohedrals U@C_{80} and Th@C_{80}, which stabilize the molecule; their molecular structure have been elucidated as isomer 28324 (C_1) by single-crystal X-ray diffraction [2]. Here we report the theoretical study of molecular structure of the non-IPR isomer 28324 (C_1) of fullerene C_{80}. According to our theoretical approach [3,4] we determined for the first time positions of single, double and delocalized π-bonds in the molecule of this isomer that was supported by our DFT calculations. Moreover we found some structural features of this lowest-symmetry molecule of the isomer. Most important is clustering of six phenalenyl-radical substructures including one pentalene (pair of fused pentagons) fragment. Such a combination of radical substructures plus overstrain of molecule because of pentalene fragment [1-3] is evidently the reason of its instability. The experimentally determined different sites of thorium or uranium atoms inside the fullerene molecules [2] are close to the aforementioned clusters that support our argumentation. As one of mechanisms of the synthesis of these non-IPR fullerene endohedral derivatives we suppose the addition of the plasma electrons to the highest spin densities positions of cage precursors, that form a stable ionic pair metal-cage precursor, than finally closing of the fullerene cage.

The reported study was funded by Russian Foundation for Basic Research, research project No.18-29-19110mk.

P9. Polystyrene and Poly(ethylene glycol)-b-Poly(ε-caprolactone) Nanoparticles with Porphyrins: Structure, Size, and photooxidation Properties

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The transport of a photosensitizer to target biological structures followed by the release of singlet oxygen is a critical step in photodynamic therapy. We compared the (photo)physical properties of polystyrene nanoparticles (**TPP@PS**) of different sizes and self-assembled poly(ethylene glycol)-*b*-poly(ε-caprolactone) core/shell nanoparticles (**TPP@PEG-PCL**) with different lengths of copolymer blocks. The singlet oxygen was formed inside both nanoparticles after irradiation with visible light. Its kinetics was controlled by the size of **TPP@PS, and TPP@PEG-PCL;** its lifetime (τ_Δ) increased with increasing nanoparticle size. The prolongation of the singlet oxygen-sensitized delayed fluorescence kinetics was found for **TPP@PS** of high size**.** The delayed fluorescence in oxygen-free conditions originating from triplet-triplet annihilation indicated a high mobility of TPP in the **PCL** core in comparison with fixed molecules in the **PS** matrix.

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P10. Encapsulation of hydrophobic bioactive substances in biodegradable polymersomes

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The entrapment of hydrophobic macromolecules in polymersomes is an important issue in the field of drug delivery. Encapsulation increases the solubility of drugs in water and enhances their bioavailability. For this reason, the encapsulation process is often studied. However, the amounts of the encapsulated substance in the membrane of polymeric vesicles are still not satisfactory.[1]

In the first part of our work we focused on preparation and characterization of polymeric vesicles. To obtain stable drug carriers of a well-defined size, we applied a biodegradable amphiphilic block copolymer. Vesicle preparation was carried out by dissolving the copolymer in a mixture of organic solvents (dimethyl sulfoxide (DMSO) and ethanol), which were then removed via dialysis against water or phosphate buffered saline. To characterize the size and stability of the polymeric carriers, dynamic light scattering (DLS) measurements were used.

In further steps, we performed the spectral characteristics of hydrophobic drugs and estimated their binding constants to the polymersomes. To calculate the amount of entrapped substance, drug loading capacity (DLC) parameters were determined. In addition, the kinetics of cargo release from the polymeric vesicles were investigated. The physicochemical properties of the polymersomes with encapsulated drugs were also examined and compared with those of empty polymersomes.

Our preliminary experiments show that small, stable polymersomes can be obtained. Spectral analyses confirm the effective entrapment of bioactive substances. The biodegradability of the polymer and the use only of low-toxic organic solvents increase chances for using these structures in pharmacy or biotechnology as carriers of hydrophobic drugs.

Acknowledgements. The authors thank the National Science Centre Poland for funding the project (grant number **DEC-2016/07/B/ST5/00250**

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P11. Trimethylamine oxide detection in solutions using surface-enhanced Raman spectroscopy

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Today, cardiovascular disease and insult are some of the most common causes of death. One of the factors of their occurrence, according to many researchers, is trimethylamine oxide (TMAO). This substance is produced in the liver from trimethylamine and in case of intestinal diseases can dramatically increase its concentration in the blood (from 0.2 mg/l to 1.5 mg/l), increasing the risk of complications [1].

In this work, the surface-enhanced Raman spectroscopy (SERS) method was used [2]. For research, substrates with the following planar SERS structure were used: Si plate; Ag reflective layer 100 nm; transparent SiO_2 insulator layer; a layer of disk-shaped Ag nanoparticles with an average diameter of ~ 40 nm. The analytes were aqueous solutions of TMAO micro, mile, and normal concentration. The application of the samples to the substrate was carried out with a 3 ml measuring pipette. The studies were carried out on a LabRAM HR Evolution Raman spectrometer at wavelengths of 514 and 633 nm, in the Raman shift region from 100 to 3500 cm^{-1}. To process the obtained spectra, the KnowItAll Academic Edition program was used.

The obtained spectra demonstrated a number of characteristic peaks of TMAO (220, 480, 750, 940, 1000, 1440 and 2940 cm^{-1}), corresponding to those in the literature. However, peaks of adsorbed substances (820-890 and 1380 cm^{-1}), soluble salts and substrate material (520 and 950 cm^{-1}) are also present on the plots. Experience shows that the most detailed spectra are obtained in the study of weakly concentrated solutions of TMAO. We have not yet been able to explain this effect. All this indicates the real possibility of using SERS for the rapid analysis of solutions for the presence of TMAO, as well as the need to improve the methodology for the preparation and study of samples.

This work was financially supported by the grant of President of the Russian Federation (project MK-2222.2019.8).

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P12. Peculiarity of internal friction in nanocomposites multiwalled carbon nanotubes and polyethylene, polyvinyl chloride, expanded polystyrene

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A non-destructive method for the technological control of the structure defects by measuring internal friction (IF) Q^{-1} was developed.

The measuring error of IF measuring was $\Delta Q^{-1}/Q^{-1} \approx 10\%$ and the elastic module relative changing was $\Delta E/E \approx 0,1\%$ [1].

The depth of the broken layer h = 1000÷3000 nm is on fig. 1.

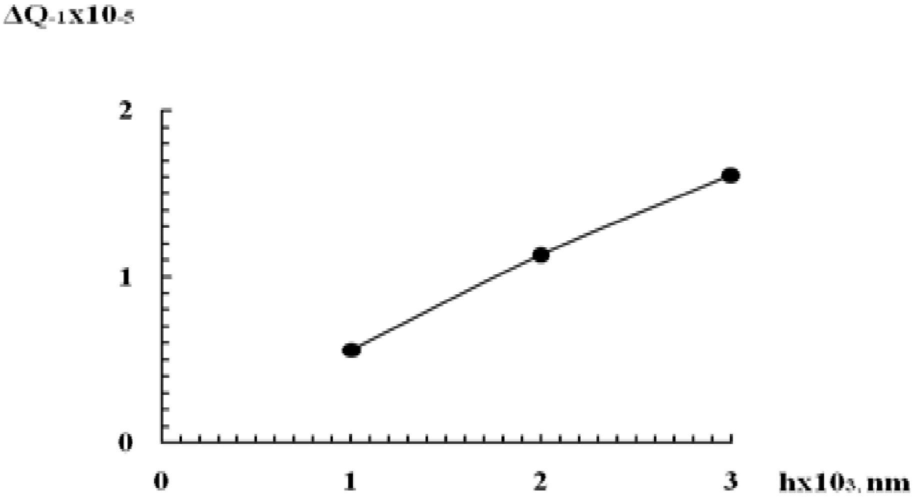

Figure 1. *Dependence of internal friction difference* ΔQ^{-1} *of* SiO_2*+Si plate from the depth of the broken layer h.*

CONCLUSIONS

1. The measuring of internal friction background Q^{-1}_0 after different heat, mechanical, radiation treatments gives information about the changing of the thermoelastic strains fields σ_i in SiO_2+Si plates.

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P13. Finite element modeling of the thermal effect on the behavior of polymers under high pressure torsion process

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The high pressure torsion (HPT) is an efficient process to obtain enhanced microstructures via super-plastic deformation. In view of its optimization, it is of prime importance to assess the relationships between processing conditions and material flow. More precisely, detailed knowledge of the plastic strain distribution in the deformed material in relation to HPT processing variables is very useful. In this context, the present work is focused to highlight the effects of the temperature and the sample thickness on the plastic strain distribution into the deformed material during HPT process. To this end, the material parameters of an elasto-viscoplastic phenomenological model were derived from compressive tests at different temperatures and strain rates on a typical thermoplastic polymer (high density polyethylene (HDPE)). The distribution of the equivalent plastic strain, the pressing force and the torque required were analyzed. Recommendations on process conditions were proclaimed at the end of this work.

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P14. Nanoscale ferroelectricity in pseudo-cubic sol-gel derived barium titanate - bismuth ferrite ($BaTiO_3$-$BiFeO_3$) solid solutions

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$BiFeO_3$ (BFO) is one of the perspective multiferroic to potentially substitute of the currently widely used $PbZr_xTi_{1-x}O_3$ solid solution. BFO has enormously high polarization in the form of thin films, which is promising for the achievement of the high piezoelectric response. The critical problem of BFO is a large leakage current significantly reducing applications. $BaTiO_3$ (BTO) and BFO solid solution is promising to stabilize the structure and improve overall piezoelectric performance of the ceramics. In this contribution, structure and piezoelectric properties of the BTO-BFO solid solutions prepared using citric acid and ethylene glycol assisted sol-gel synthesis method were studied. Depending on the dopant content the samples are characterized by tetragonal, tetragonal-pseudocubic, pseudocubic and rhombohedral structure as confirmed by X-ray diffraction measurements. Thought an increase of the BFO content leads to a reduction in the cell parameters accompanied by an elimination of the polar distortion of the unit cell, non-zero piezoresponse was observed in the compounds with pseudocubic structure. A coexistence of the nanoscale regions having polar and non-polar character is considered as a key factor resulting in local and macroscopic piezoresponse.

The research 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, refs. UIDB/50011/2020 & UIDP/50011/2020, financed by national funds through the FCT/MEC, and project TransFerr, European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie, grant agreement No. 778070.

P15. In-plane polarization contribution to the vertical piezoresponse force microscopy signal mediated by the cantilever "buckling"

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Rigorous experimental/theoretical approach to measure and minimize in-plane piezoresponse contribution to the vertical piezoresponse force microscopy (PFM) signal is introduced. The in-plane piezoresponse mediated by the cantilever "buckling" is shown to affect the apparent vertical PFM signal being of the same order of magnitude as a true out-of-plane piezoresponse. We found that the common set-up of the PFM mode with the laser beam focused close to the cantilever free end is susceptible to the combination of the in-plane and out-plane piezoresponses. Therefore, the vertical piezoresponse phase depends on the orientation of the polarization in the individual grains and domains. Decoupling of these two contributions based on a simple mathematical procedure is demonstrated.

Additionally, the row PFM data are analyzed as a function of the laser beam focus position on the cantilever and the position allowing suppressing the "buckling" contribution and hence measuring only the out-of-plane piezoresponse component is revealed. This approach can be used for the accurate recovery of the piezoresponse displacement vector, what is of paramount importance for the reconstruction of the domain structures and quantitative characterization of the polarization distribution and local piezoelectric properties in ferroelectric materials.

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).

P16. Mechanical properties and thermal conductivity of epoxy composite containing aluminum-exfoliated graphite nanoplatelets hybrid powder

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In this work, epoxy/aluminum-exfoliated graphite nanoplatelet (epoxy/Al-xGnP) composites were prepared. Before compounding, two types of Al-xGnP hybrid powder were prepared, one is fully embedded xGnP and the other is partially embedded xGnP in aluminum. TEM images of hybrid powder showed the partially and fully embedded xGnP in aluminum. The thermal conductivity of epoxy composite increased with the increasing Al, xGnP and Al-xGnP content. Compared with the epoxy composites containing Al and x-GnP, the epoxy composites containing Al-xGnP hybrid powder showed synergistic effect on the thermal conductivity. Especially, partially embedded epoxy/Al-xGnP composite showed the highest values of thermal conductivity at the same filler concentration. The tensile strength of epoxy composites decreased with the filler content. The tensile modulus of epoxy composites increased with the filler content. In the mechanical properties, fully embedded epoxy/Al-xGnP composite showed better results than partially embedded epoxy/Al-xGnP composite.

P17. Solid phase synthesis of calcium stearate on modified screw equipment

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For the first time, the technology [1] of solid-phase synthesis of calcium stearate was developed under conditions of low-temperature (up to 100 °C) and mechanical force action associated with the application and subsequent relaxation of the stress field on the reaction mixture of the trimolecular reaction of stearic acid and calcium hydroxide. Under the conditions of mechano-energetic impact in a modified screw apparatus, providing effects on the reaction mixture of continuous plastic deformations, various kinds of defects are formed on the surface of the molecules of the reactants, expressed in the anisotropy of the crystal lattice. Hydrogen bonds arising in carboxylic acids are among the strongest among other hydrogen bonds; their energy is 29 kJ / mol [2]. At the same time, the electron density is shifted towards the most electron-withdrawing oxygen atom of the carbonyl group. Mechano-energetic effect leads to a weakening of the bond between oxygen and hydrogen in the hydroxyl group and ease of cleavage of the hydrogen atom from the hydroxyl in the form of a proton (H +), which is expressed by mass transfer at the interface between the heterogeneous heterophase reaction.

The use of an extrusion apparatus with one or more satellite augers provides, firstly, the maximum degree of dispersion of the components of the reaction mixture, and secondly, an unprecedentedly large area of the interface between the reagents and the topochemical reaction.

The time of product synthesis during the liquid-phase process is reduced, in the case of the non-catalytic process, from several hours to 2.28-10 minutes, depending on the configuration of the extrusion equipment. The samples obtained by the solid-phase method were characterized by a high efficiency of the stabilizing action and corresponded to the standards of industrially manufactured products.

Such conditions, recreated in the laboratory installation of a screw apparatus, provide for intensification of the technological process, energy-saving and environmental safety.

The influence of mechanical energy effects: pressure and plastic deformation on the process of solid-phase synthesis of calcium stearate inside the extruder cavity was shown [3].

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P18. Improvement of active layers homogeneity for the MEA's (Membrane Electrode Assembly) of PEMFC (Proton Exchange Membrane Fuel Cell): impact of the ink quality formulation

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Purpose:

The French Atomic Energy and Alternative Energies Commission has been working for many years on PEMFC Proton Exchange Membrane Fuel Cells, this technology which could be the future of electric cars. The goal is to improve the performance and durability of PEMFC. This study will deal with the quality of the ink that can be used to print by coating process, the active layers for Membrane Electrode Assembly MEA.

Some research has demonstrated the impact of the active layer's homogeneity on fuel cell performance (*impact of solvents* [1], *impact of printing processes* [2]). In our case, the aim is to obtain homogeneous active layer after coating deposition process by studying the formulation: the order of introduction of components and the dispersion processes.

Moreover, the study will handle with the impact of agglomerates present on the active layers for the fuel cell's performance.

Materials & Methods:

Catalytic ink is used in the study. **Two dispersion methods** were tried including low shear mechanical (magnetic agitation) to high shear mechanical mixers (mixers from Dispermat® and Silverson®) and planetary mixers (Mazerustar from Kurabo® and Kakuhunter from Sodipro®).

In order to characterize the quality of the ink and the presence of agglomerates, several techniques were used: **rheometer** (ink rheology), **electro-acoustic probe** (size of particles), **grind gauge** (maximum size of particles), and active layers made with the **coating** method and observed with the **scanning electron microscope (SEM).**

Results:

After having carried out several formulations applied to coating process, three of these formulations were chosen and enable to have less agglomerates in active layers.

A comparison was made between different dispersion processes thanks to characterization. Planetary mixer seems to be the best method to have smallest particles into inks and to obtain homogeneous layers. Impact of time is also shown through this study with a better quality of deposit few days after the mixing.

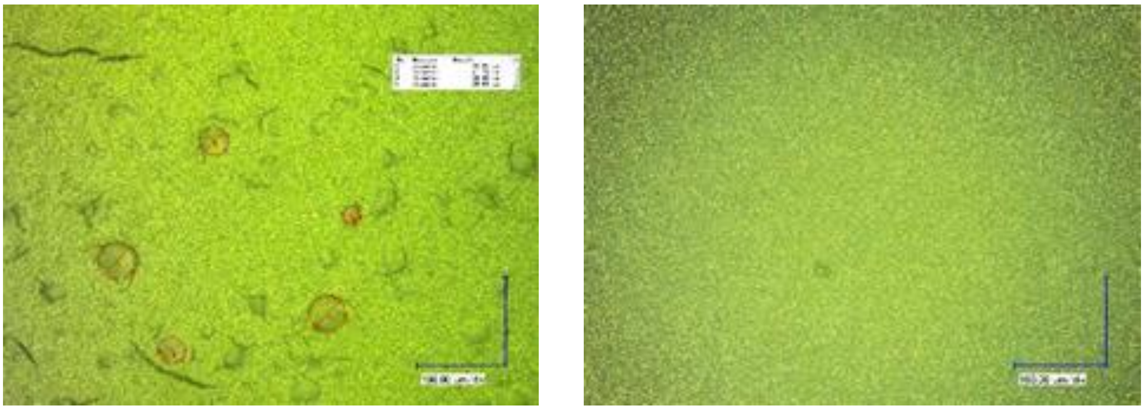

Figure: Active layer deposited by coating process and observed under an optical microscope with 500x magnification. Left: ink dispersed with a high shear mechanical mixer; Right: ink dispersed with a planetary mixer

Conclusion & Perspective:

Different formulations, for use coating process, have been made with different dispersion processes. Several of them have distinguished themselves by the quality of the mixture leading to reach an average of ink particle size submicron, and by the homogeneity of the coated active layer obtained (no agglomerates observed on cross section).
This study must be completed by the impact of agglomerates onto performance and durability and could also be used for other printing method as screen-printing process.

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P19. Effect of adding titanium dioxide (TiO_2) on the mechanical behavior and corrosion resistance of hydroxyapatite sol–gel thin coatings on 316 L stainless steel: *Biomedical application*

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Hydroxyapatite (Ca10(PO4)6(OH)2, HAP) is widely used for hard tissues repair due to its chemical and structural similarities with the mineral phase of bone and teeth. In this study we investigated the effect of the addition of TiO2 inner-layer on the morphological and mechanical properties of hydroxyapatite (HAP) bioceramic coatings deposited on 316L stainless steel by sol-gel method in order to improve the properties of hydroxyapatite and expand its clinical application
we have noticed that thin films of HAP/TiO2 on 316L SS possess combined advantages of biocompatibility and corrosion-resistant properties. we recall that the indentation hardness is often used as an initial guideline for the qualification of a coating for any application requiring wear resistance. intrinsic film hardness can be directly measured when the penetration depth of the indenter is lower than 10% of the coating thickness. In our study, The deposition of the inner-layer have provided the formation of new types of hydroxyapatite coatings. Classical hardness measurements conducted on the coated systems under the same indentation load (10g) indicates that the microhardness of the HAP coating is improved by the addition of TiO2 inner-layer on the 316L stainless steel substrate, the adhesion to the steel is also improved. We notice that the hardness is comparable with those of natural teeth . The corrosion resistance of the 316L stainless steel in simulated body fluid (SBF) was found to increase after the deposition of the HAp and HAp/TiO2 coatings as confirmed by the cyclic voltammetry test.

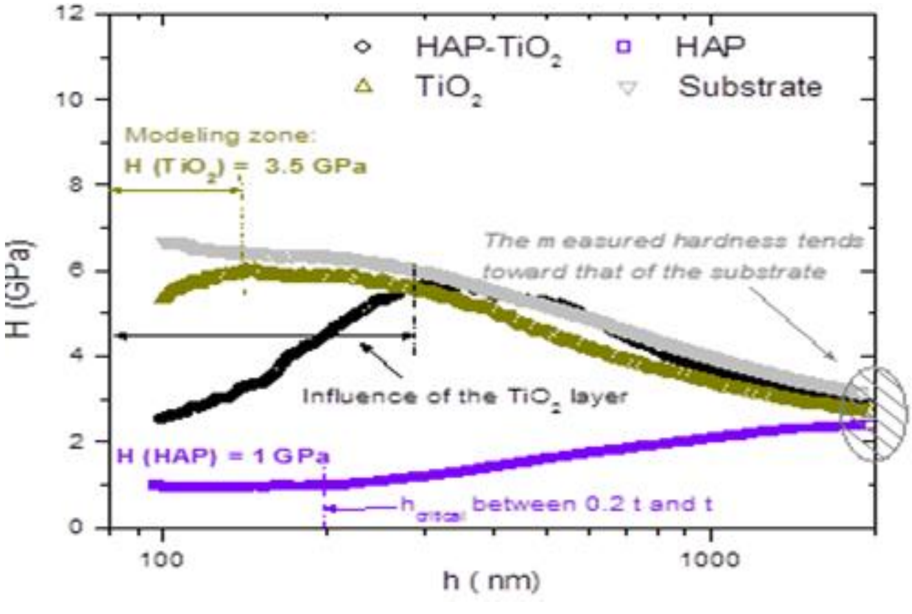

Fig.: Hardness versus the indenter displacement obtained by using the CSM mode of nanoindentation performed on the uncoated substrate, the HAP, TiO_2, and HAP–TiO_2coatings

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P20. Photoelectrochemical properties of anodic WO_3 sensitized with $CuWO_4$

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In order to obtain anodic tungsten oxide with enhance photoelectrochemical properties in visible light and narrow band gap, oxide layers were sensitized with $CuWO_4$ by impregnation in $Cu(CH_3COO)_2$ solution for 1 h, 5 h, 10 h or 24 h and then annealed at 500 ^oC to create a heterojunction. As-received samples were subjected to characterization of the morphology, composition, photoelectrochemical and semiconducting properties by scanning electron microscope (SEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction analysis (XRD), Raman, photoelectrochemical (PEC) and Mott-Schottky measurements. Although the photoelectrochemical response in the UV range and estimated donor density from Mott-Schottky measurements drop significantly after impregnation due to insufficient separation of charge carriers in the $CuWO_4/WO_3$ heterojunction, a beneficial improvement in photoelectrochemical response was observed in the visible light. In particular, an increase in generated photocurrents and reduction in band gaps with prolonged impregnation time were observed. It was found that anodic WO_3 sensitized with $CuWO_4$ exhibits improved semiconducting and photoelectrochemical properties in the visible light region compared to unmodified tungsten oxide layers. The photoresponse in UV light of $CuWO_4/WO_3$ samples might be enhanced in the future by loading the material with noble metal nanoparticles such as Cu, Ag, or Au, which will improve charge carriers separation.

P21. Enhanced photocatalytic activity of TiO_2-Ag and TiO_2-Au formed on a stainless steel mesh

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Currently, photocatalytic materials are actively used to solve various environmental and energy problems. It is known that TiO_2 based materials decompose almost any organic compound. However, the use of titanium dioxide in its pure form demonstrates low efficiency. Nanostructuring and modification by various elements perfectly improve the photocatalytic activity of TiO_2 materials. In this work, the features of electrophoretic deposition of TiO_2 materials, the effect of modification by Au and Ag metal particles on the photocatalytic activity are considered.

The TiO_2 electrophoretic deposition was carried out on a stainless steel mesh from a suspension based on isopropyl alcohol, a TiO_2 nanopowder (particle size 20 nm), and a surfactant. Au and Ag particles on the TiO_2 surface were formed by vacuum thermal evaporation. The surface morphology, thickness, and stoichiometry of the obtained samples were studied by scanning electronic microscopy and energy dispersive X-ray analysis. The samples' reactivity was investigated based on the activity of carbon dioxide photoreduction. The quantitative and qualitative gas analysis was performed on a gas chromatograph with a flame ionization detector. It was found that the CO_2 photoreduction reaction occurred with the formation of methanol, methane, and isopropanol.

This work was supported by the Russian Science Foundation (project No. 19-19-00595).

P22. Study of the TiO_2/Me structure by IR spectroscopy for use in photoactive fuel cells

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TiO_2-based fuel cells attract much attention from the scientific community due to the photocatalytic reduction of CO_2 in the presence of water to methane and its homologous [1]. However, pure TiO_2 shows low efficiency. Increased efficiency can be achieved by alloying [2]. One of the modification methods is the formation of an array of plasmonic metal nanoparticles on the surface of TiO_2.

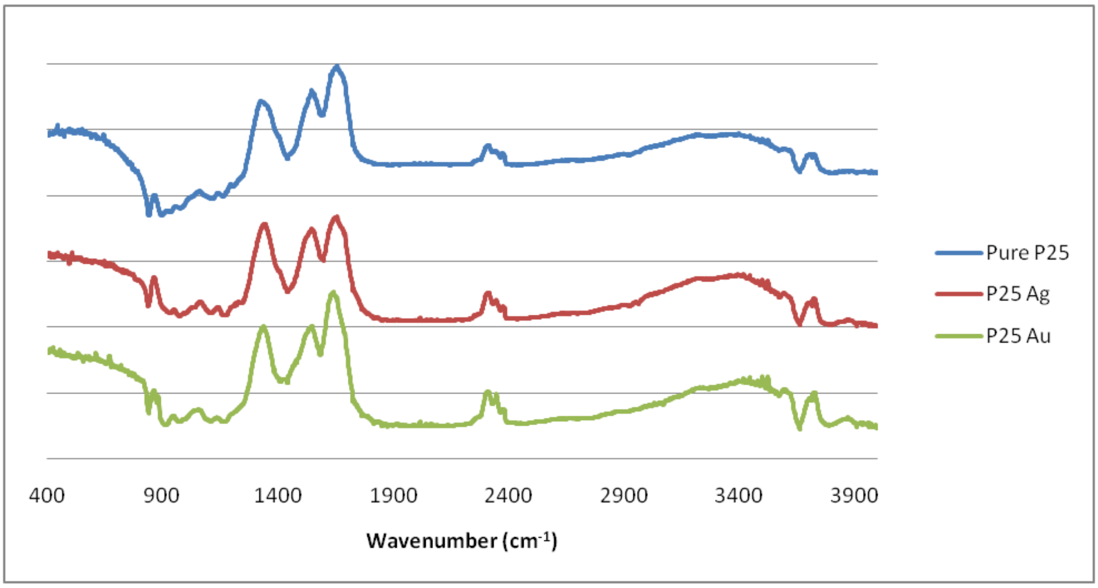

Fig. 1. IR spectra of CO_2 photoreduction on TiO_2 under UV irradiation after 20 minutes for TiO_2, TiO_2/Ag, TiO_2/Au

A TiO_2 “Degussa P25” was deposited on a stainless foil substrate by electrophoretic deposition. After application, the samples were annealed in vacuum. The method of vacuum-thermal evaporation was used to modify the surface with an array of Au and Ag nanoparticles. The studies were carried out by diffuse reflective infrared spectroscopy with Fourier transform under the influence of ultraviolet radiation. The measurements were carried out in a gas mixture stream of 1% CO_2.

The presence of an additional OH group peak in the region of 3900 cm^{-1} was observed on samples with Au and Ag nanoparticles. An increase in the intensity of individual peaks was also observed, which tells us about the increased activity of the modified samples.

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

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P23. Improved performance of Silicon solar cells by ZnMgO front layer

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Silicon solar cells play a dominant role in the photovoltaic market. However, their manufacturing process is quite expensive and involves complex processes. Therefore, new materials must be explored for the manufacture of potentially higher efficiency and lower cost solar cells.

ZnMgO alloy is a very promising transparent conductive oxide layer (TCO) and which acts as front layer as well as an anti-reflective coating in silicon solar cells reducing costs and complexity of process.

Numerical simulation using the 1D-SCAPS software enables to find the optimized parameters of crystalline p-Si/ZnMgO front layer and compared to structure with ZnO layer. The result shows conversion efficiency of 16.57%. This result is due to stress caused by the high lattice mismatch at the ZnMgO / Si interface. The introduction of a thin layer of hydrogenated amorphous silicon improves the cell output performance.

P24. Characterization of nanostructured tin oxide obtained by galvanostatic anodization

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In recent years, nanostructured tin oxide has gathered great attention due to its unique properties that make it an excellent candidate to be used, e.g., as an electrode in solar cells, photoelectrochemical water splitting, or energy storage devices [1,2]. One of the most promising methods used for the synthesis of nanoporous SnO_x is anodic oxidation of metallic tin. Although different conditions that lead to obtain continuous and crack–free nanoporous layers with a thickness up to tens of microns were proposed, new approaches still need to be investigated to improve semiconducting properties of such kind of films. For this reason, in this work, we present some preliminary results on the galvanostatic anodization of tin in various electrolytes and difference in photoelectrochemical properties of generated tin oxide films when compared to materials obtained under potentiostatic regime. Morphology and material composition were investigated by FE-SEM, EDS, and XRD. Moreover, semiconducting properties were verified using photoelectrochemical measurements and UV-VIS spectroscopy.

Acknowledgments

The research was supported by the Polish Ministry of Science and Higher Education (Project no. 0196/DIA/2018/47).

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P25. Reactions of $BaTiO_3$ with LiH: trapping different stages of $BaTiO_3$ reduction

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As an important mixed-anion compound, oxyhydride materials[1] have been researched extensively for their unique electronic properties and potential application in catalyses. We investigated the hydride reduction[2] of tetragonal $BaTiO_3$ using LiH. The reactions employed molar H:$BaTiO_3$ ratios of 1.2, 3, and 10 and variable temperatures up to 700 °C. The air-stable reduced products were characterized by powder X-ray diffraction (PXRD), scanning electron microscopy, thermogravimetric analysis (TGA), XRF, and ^1H magic angle spinning (MAS) NMR spectroscopy. Effective reduction, as indicated in the formation of dark blue to black colored, cubic, products was observed at temperatures as low as 300 °C. Their lattice parameter were in a range between 4.005 Å and 4.022 Å. At 700 °C LiH reduction of $BaTiO_3$ yielded a mostly amorphous product. The product obtained at 300 °C corresponded to a stoichiometric oxyhydride, $BaTiO_{2.9}H_{0.1}$, whereas reduction at higher temperatures resulted in simultaneous O defect formation, $BaTiO_{2.9-x}H_{0.1-x}$, and eventually – at temperatures above 450 °C – to samples void of hydridic H. Concomitantly, the particles of samples reduced at high temperatures (500 – 600 °C) show substantial surface alteration, which is interpreted as the formation of a $TiO_x(OH)_y$ shell, and sintering. The band gap, as obtained from UV-VIS spectroscopy and Mott-Schottky analysis showed detailed energy structure of the materials, which showed potential application in catalysis of water[3].

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P26. Photoluminescence and EPR studies of single diamonds with GeV-color centers formed by ion implantation

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At present, a large number of color centers in the diamond which could be used as single-photon sources are known. These include color centers such as NV-, SiV-, SnV-, NE8-centers, etc. [1]. However, among these color centers, only NV- and SiV-centers show reproducible results. Recently, room-temperature photoluminescence of GeV-centers had been observed in the diamond implanted with Ge ions at energy ranged from 150 to 260 keV [2]. The single photon emission capability of GeV-center with a ZPL line at around 602 nm had been demonstrated at first time. In the given work, Ge^+ ions were implanted in single crystalline (001)-face oriented plates of synthetic diamond (type IIa, *NDT Ltd)* at more low energy of 40 keV and the fluences in the range of (0.05-1.0) $\times 10^{15}$ ion/cm^2. The implanted diamond plates were then annealed at high temperature of 1273 K under high vacuum conditions (10^{-9} mbar). A home-made confocal microscope and laser diode excitation at a wavelength of 520 nm were used to look for GeV-centers in diamond. The spectra of photoluminescence (PL) was taken at room temperature. In addition to the intense Raman line (558.6 nm), PL spectra are characterized by a narrow emission line at a wavelength of 601.5 nm related to GeV-centers. Electron paramagnetic resonance (EPR) was used to determinate the structural position and the crystalline symmetry of GeV-centers under study. However, EPR spectra reveal only one non-structured line with g-factor of 2.003 (except very weak lines from NV-centers) at room and liquid nitrogen temperatures in both rf X- and Q-bands. Moreover, there not angular dependence of EPR spectra on the orientation of diamond crystalline plate with respect to magnetic field direction. The last suggests that the GeV-center has a more symmetrical position in crystalline structure of diamond than, for example, a SiV-center similar to it (point symmetry D_{3d}).

This work was supported by the Mega-grant of the Government of the Russian Federation (Agreement No. 14.W03.31.0028).

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P27. Optical parameters study of amorphous germanium (α-Ge) by spectral ellipsometry

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At ion implantation of Ge a porous layer is formed on its surface the thickness of which is several times more than the average ion range [1]. The possibility of creating a nanoporous structure on the Ge surface has led to a trend in recent years for the use of Ge in new areas of technology: in lithium-ion batteries as an anode material, as new materials for gas sensors and optoelectronic devices. As previously shown by the example of single-crystal silicon (c-Si) implanted with various types of ions in a wide energy range, spectral ellipsometry (SE) is an informative technique for studying partially amorphized semiconductor layers [2, 3]. This work presents the dispersion dependences of the optical parameters of α-Ge obtained by the study results of a thick film of α-Ge (1000 nm) grown by magnetron sputtering technique on a corundum substrate. These dependencies were used for SE study of c-Ge plate implanted with fluence 4×10^{16} ion/cm^2 of argon ions 300 keV energy. The established value of the disordered layer (amorphous layer) thickness during ion irradiation corresponds to the thickness of the layer obtained by simulating irradiation in the SRIM-2008 program [4].

The reported research was funded by Russian Science Foundation (grant No 19-79-10216).

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P28. Fluorescence properties of Nd-doped ZnO thin films obtained by the sol-gel method

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Recently, considerable attention has been paid to metal oxide wide-gap semiconductors, such as ZnO, TiO, SnO_2 and In_2O_3 doped with rare-earth ions (REI). Therefore, new hybrid materials characterized by unique optical properties were obtained exactly by doping with REI metal oxides.

In the present study, the $ZnO:SiO_2$ films doped with Nd^{3+} (0.5 - 7% wt.) were synthesized by the sol-gel method [1]. Further their optical characteristics were analyzed by absorption and fluorescence spectroscopy, whereas the surface morphology - by scanning electron microscopy. It was found that the luminescence intensity (λ_{ex} = 280 nm, λ_{ex} = 361-363 nm) decreases in the samples with a low (0.5 and 1% wt.) content of Nd^{3+} in the film by 21% and 43%, respectively, in comparison with unmodified $ZnO:SiO_2$ films. While a subsequent increase in the amount of neodymium to 5–7% resulted in a luminescence rise by 11–29%. The intrinsic luminescence of Nd^{3+} in the film was observed at 586 nm. It is worth noting that the dependence of the intensity on the amount of dopant is nonlinear. However, all tests showed an increase in luminescence in 1.4 - 5 times along with the amount of dopant in the film.

This publication has been prepared with the support of the "RUDN University Program 5-100". This work was supported by the competitiveness program of NRNU MEPHI.

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P29. Effect on Morphology due to Dopant Elements, and Morphology-Dependent Photocatalytic Activity of ZnO Nanomaterials

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In nanotechnology, various morphologies are grabbing contemporary attention for various applications [1]. We report controlling rods and flowers novel morphologies in ZnO based nanomaterials with the help of Co and Sn dopant [2, 3] respectively, developing effective (0.01M%, 0.02M%, and 0.03M%) doping percentage strategies. For the synthesis of pure and doped ZnO nanomaterials were used zinc nitrate, hexamethylenetetramine, cobalt chloride, tin chloride as the starting materials in simple wet chemical co-precipitation methods at 90° C for 3 hours. The crystallite size found by X-ray diffraction spectra in the range of 26-37 nm. The morphological transformation of nanostructures is revealed gaudily through scanning electron microscopy and transmission electron microscopy spectrograph due to the dopant incorporation. Interestingly, the morphology of nanostructures develops with increasing percentage of dopant concentration in ZnO. Calculated band gap 3.1-3.3 eV observed by UV-Vis spectra. Decreeing in defects and oxygen vacancy analyzed from weak UV and strong visible emission spectra by photoluminescence. The experiments revealed that the flowers structures shown enhance photocatalytic activity as compare to rods structures.

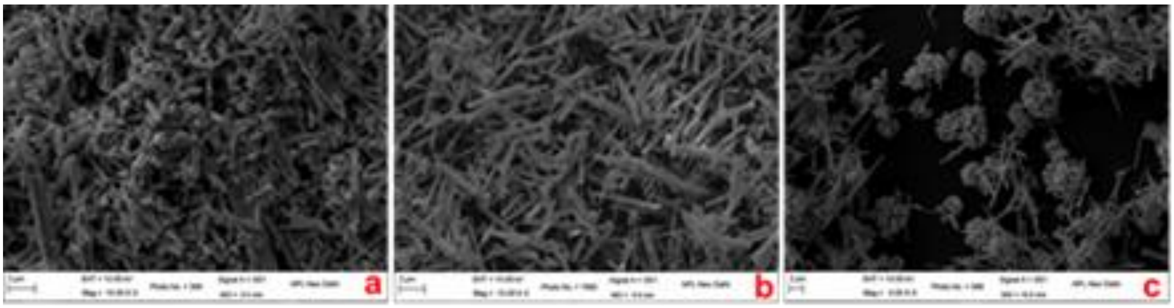

Figure- SEM images of (a) Pure ZnO, 0.03M% (b) Co and (c) Sn doped ZnO.

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P30. Theoretical and Experimental Properties of Ag_2SeO_3 Crystals

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Selenium-Silver based matrices exhibit interesting structural, optical and photoluminescent properties, which accounts for a great potential material in many research fields like physics, chemistry and materials science. Moreover, the chemistry of Selenium and Silver is very prominent in biological systems due to in part from their interaction with molecules like proteins. In this work, Silver Selenite (Ag_2SeO_3) were prepared by the Coprecipitation method, which is a fast, simple, and efficient experimental procedure to prepare inorganic materials. X-ray powder diffraction patterns results showed intense and sharp peaks which could be indexed to the pure monoclinic phase and $P2_1/c$ space group, attesting that materials are pure and present long-range order. It was also observed defined experimental Raman modes which corroborated to the theoretical ones calculated indicating short-range order. The morphology was confirmed by FE-SEM microscopy and Wulff construction, showing cubic-like rods of different width and length. PL spectroscopy showed an intense band in the visible region with maximum at around 700 nm. The geometry, electronic properties of the bulk, and surface energies of these materials were evaluated using first-principles quantum mechanical calculations based on the density functional theory (DFT/B3LYP) to provide information at the atomic level. In this sense, experimental results were correlated to theoretical studies and enabled a deep understanding between structure and property. Inspired by the above considerations, these materials may present superior characteristics for new compounds with photoluminescence applications.

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P31. Structural and optical properties of the Ag-Cu composite nanoparticles

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Plasmonics of metal nanoparticles, which is based on the phenomenon of localized surface plasmon resonance (LSPR), is a rapidly growing and expanding field of research due to wide prospects for its use [1, 2]. In order to expand the spectral capabilities of the SERS method, Ag-Cu alloy nanoparticle arrays were studied. Arrays of Ag-Cu nanoparticles were formed by vacuum thermal evaporation and condensation on an unheated substrate followed by heat treatment at 230 °C. A higher Raman scattering enhancement in the red region of the spectrum when using an array of nanoparticles of the Ag-Cu eutectic system was found. This enhancement is comparable to the one of pure silver particle array in the blue region of the spectrum. Transmission electron microscopy study has shown that the feature of the Ag-Cu array is that many particles are composite: one part consists of copper, and the other part is made up of silver. These parts have a perfect (possibly heteroepitaxial) boundary. It is believed that the localized surface plasmon resonance excited in the copper part by red light can be transmitted without any loss into the silver part, while the one excited in the silver part by blue light, quickly fades out in the copper part, because blue light has a higher frequency than the copper plasma frequency.From the point of view of SERS applications, the use of Ag-Cu particle arrays allows extending the advantage of silver to the red region of the spectrum.

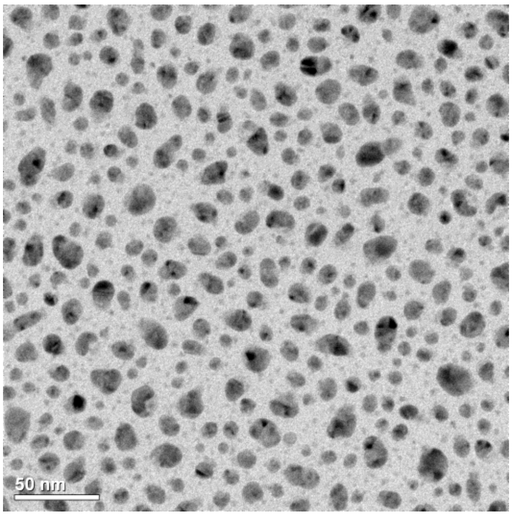

Fig. 1. TEM image of silver Ag-Cu nanoparticles arrays.

This work was supported by the State assignment 2020-2022 № FSMR-2020-0018 (Proposal mnemonic code 0719-2020-0018).

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P32. The influence of selected cationic derivatives of phosphatidylcholines on the properties of model mammalian membranes

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In recent years, many studies have focused on the search the new carriers of drugs or genetic material. A relatively new class of compounds utilized in drug delivery systems is cationic lipoids. These are synthetic bioactive molecules of lipid-like structure, which causes that similarly to natural lipids they possess amphiphilic character. Many of cationic lipoids, however, show strong toxicity which hamper their *in vivo* application. Therefore novel cationic lipoids are still synthesized and investigated. The triesters of phosphatidylcholine (EPCs) are a particular group of cationic lipoids which as derivatives of natural phosphocholines exhibit significantly reduced toxicity. The exact mechanisms of lipofection and drug delivery by cationic lipoids are probably a multi-step process and so far there have been not fully elucidated. However, the biological membrane is the first place an action of these bioactive molecules either as a target or as a barrier that protects the interior of the cell.

The purpose of the research was to determine the impact of selected triesters of phosphatidylcholine on the properties of model mammalian membranes in which the molar ratio of lipids reflected their proportion in the lipid rafts. In the studies, as model systems, Langmuir monolayers and liposomes were applied.

The obtained results show that the incorporation of EPCs into model mammalian membranes leads to significant changes of their properties. These alterations mainly concern the character of intermolecular interactions. The addition of EPCs into model lipid rafts leads to the weakening of impacts between lipids. Moreover, the incorporation of cationic lipoids into model membranes increases of fluidity, disorder of *acyl* chains and permeability. The presence of cationic lipoids also reduces the membrane stability.

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P33. The study of the impact of lipid structure on their interactions with 2-hydroxyoleic acid

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The main goal of this study was to investigate the effect of 2-hydroxyoleic acid on model cell membranes of eukaryotic organisms. 2-hydroxyoleic acid is one of the potential anti-cancer drug. The previous results indicate that pharmacological effect of this substance is associated with its incorporation into cell membrane and modification of the membrane-lipid composition. The molecular mechanism of action of this substance is not completely understood.

The investigations were performed for model systems containing sphingomyelin (SM), 2-oleoyl-1-pallmitoyl-sn-glycero-3-phosphocholine (POPC) and cholesterol (Chol) as the components of cell membranes. The cholesterol content was 5, 15 and 33.3 mol%. The research was conducted with Langmuir monolayer technique with Brewster Angle Microscopy support.

The obtained results show a significant effect of 2-hydroxyoleic acid on model cell membranes. It was found that the addition of this substance leads to changes in the fluidity of the films and reduces the order of hydrophobic chains.

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P34. The influence of bisphenols on the properties of model human erythrocyte membranes

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Bisphenols are a group of chemicals widely used in the manufacturing of plastics, polysulfones and epoxy-resins. Bisphenol A (BPA) is the most commonly used analogue, however, due to its toxicity, other structurally similar bisphenol compounds have been introduced into the market in recent years. The most common are bisphenol F (BPF) and bisphenol S (BPS). Nowadays it is known, however, that this BPA analogs exert toxic effects similar to those of BPA but of different magnitude. Several studies have reported the occurrence of BPA, BPS and BPF in human specimens. Among various aspects of the toxicity of this substances, their effect on the red blood cells is extensively studied.

The aim of the presented work was to compare the effect of BPA, BPS and BPF on model erythrocyte membranes and to get insight into the origin of the differences in the harmful effect of these substances on cells. Thus, the influence of bisphenols on multicomponent Langmuir films mimicking the outer leaflet of human erythrocyte membrane was investigated. The experiments were carried out for SM/POPC/Chol system and also for particular erythrocyte membrane lipids: SM and Chol (the effect of bisphenol A, S and F on one-component POPC films has already been analysed [1]). The experiments were carried out using Langmuir monolayer technique accompanied by Brewster Angle Microscopy.

Based on the obtained results it was found that BPA and BPF affect artificial lipid membranes more strongly than BPS, by changing their stability, fluidity and morphology. However, it is worth emphasizing that BPA acts on the erythrocyte lipids more selectively than BPS and BPF and the influence exerted by this substance is more strongly determined by the membrane composition. It was also suggested that cholesterol may act as the molecule of a decisive role from the point of view of the magnitude of the incorporation and the effect of BPA and BPF on membrane. Thus, the level of bisphenols toxicity to erythrocytes may depend on the concentration of cholesterol in their membranes.

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P35. Optical and Structural Properties of $Cu_2Zn_{1-x}Cd_xSnS_4$ Thin Films Obtained by Ultrasonic Spray Pyrolysis

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Cu_2ZnSnS_4 (CZTS) is one of the most promising materials as an absorber layer in a thin film solar cell because of a suitable band gap energy of about 1.5 eV and of a high absorption coefficient over $10^4 cm^{-1}$ in the visible range[1, 2]. Recently, the synthesis of an alternative compound of $Cu_2Zn_{1-x}Cd_xSnS_4$ (CZCTS) with $(0\leq x\leq 1)$ for absorber layer thin films solar cells has been also reported [3, 4]. In this work, $Cu_2Zn_{1-x}Cd_xSnS_4$ (with x=0; 0.5 and 1) films were deposited by spray pyrolysis. copper chloride $CuCl_2$, zinc chloride $ZnCl_2$, cadmium chloride $CdCl_2$, tin chloride $SnCl_2$ and thiourea $SC(NH_2)_2$ were used as source of different elements (Cu, Zn, Cd, Sn and S). The solutions containing precursor elements were sprayed ultrasonically onto glass substrates. The substrate temperature, spraying duration and the flow rate of spraying were fixed at 350°C, 30min and 10ml/hour respectively. The formation of kesterite crystal structure of Cu_2ZnSnS_4 (x=0) and stannite structure of Cu_2CdSnS_4 (x=1) is confirmed by using XRD analysis. Raman analysis reveals the existence of Cu_2S as secondary phases in the films deposited with x= (CZTS). All films have a transmittance lower than 5% in the visible range, indicating the high absorption of the films. the optical band gaps of the films estimated from the transmittance spectra were approximately 1.37, 1.29 and 1.34 eV corresponding to the values x= 0; 0.5 and 1 respectively, which are suitables for photovoltaic applications, a minimal band gap was obtained at x=0.5 ($Cu_2Zn_{0.5}Cd_{0.5}SnS_4$).

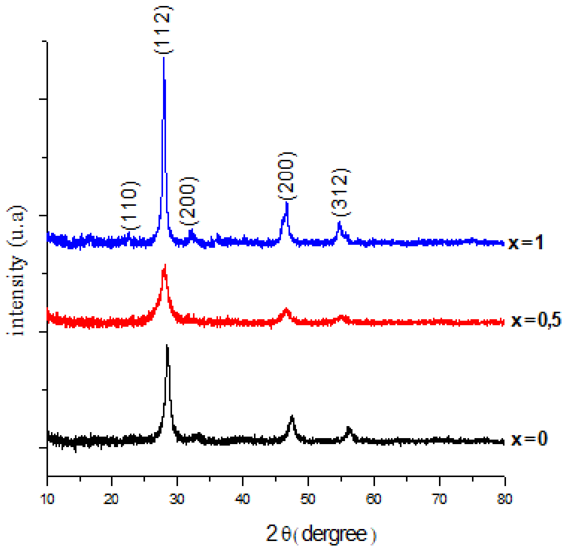

Figure 1.XRD patterns of CZCTS films

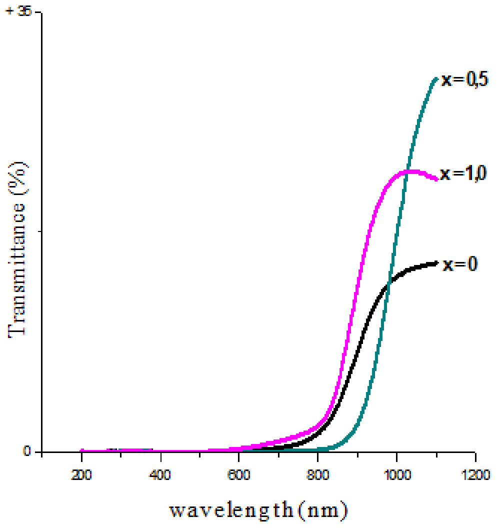

Figure2. Transmittance spectra of CZCTS films

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P36. Thermal stabilization of geometric parameters at 100°C of a silver nanoparticles array obtained by vacuum-thermal evaporation on a unheated substrate

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Methods of controlled nanoparticles formation are interesting due to many applications of them. For example, CNT’s growth, antibacterial purposes, plasmonics [1-3]. It is known that the nanoscale state for many materials significantly differs from the mass state. This article demonstrates the unusual behavior of silver nanoparticles array during annealing at low temperature. Results of investigation via the atomic force microscopy (AFM) with in-situ heating up to 200°C are presented. Object of AFM-investigation was an evolution of silver nanoparticles array formed on the surface of SiO_2 by vacuum thermal evaporation on an unheated substrate. Using of this method allows to obtain a qualitative estimate of temperature influence on the geometry of an nanoparticles array. It was experimentally shown that a sharp enlargement of silver nanoparticles and decreasing of their quantity on the surface occurs in a small temperature range of 75-100°C. In the temperature range 100-200°C there are no noticeable changes in the silver nanoparticles array. After statistical processing of the obtained data the average sizes of the formed particles and their density per unit area at each stage of the experiment were determined, the corresponding dependences were obtained.

This work was supported by the State assignment 2020-2022 № FSMR-2020-0018 (Proposal mnemonic code 0719-2020-0018)

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P37. The influence of the PEG-ylation degree of 1,2-disteroil-sn-glycero-3-phosphoethanolamine on the molecular organization of model lipid membranes

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Due to the growing importance of controlled drug delivery systems (DDS), the basic task of nanotechnology is to develop stable, effective and non-toxic nanostructures in which the drug can be encapsulated and delivered to a specific diseased site in the patient's body. Currently, one of the most popular ways to improve the physicochemical and pharmacokinetic properties of liposomes is to introduce into their structure poly(ethylene glycol) conjugated with molecules 1,2-disteroil-sn-glycero-3-phosphoethanolamine (DSPE) - polymeric stabilizer.

The aim of this work was to investigate the influence of the PEG-ylation degree of DSPE (DSPE-PEG350 and DSPE-PEG750) on the properties of monolayers and lipid bilayers of lipids naturally found in animal cells such as cholesterol, phosphatidylcholine (POPC) and sphingomyelin (SM) and POPC/SM/Chol = 1: 1: 1 whose composition reflected the structure of the lipid rafts in the membranes of animal cells. During the studies were used Langmuir monolayers and liposomes as a model of biological membranes, which enabled the optimization of physicochemical properties of potential carriers of therapeutic substances. The liposomal formulations were researched with using of Dynamic Light Scattering, zeta potential measurements and Spectrofluorymetry which allowed for following the release of calcein encapsulated in liposomes and changes of fluorescence anisotropy of DPH.

The obtained results proved that the molecular organization of the model lipid monolayers strongly depends on the degree of PEG-ylation of poly(ethylene glycol) conjugated with DSPE. Moreover, the addition of a stabilizer with different length of polymer chain changes the stability, permeability and anisotropy of the formed liposomes.

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P38. An Investigation on 100 MeV Ni7+ Swift Heavy ion Irradiation effect on the Ferroelectric Triglycine Sulphate <011> Oriented Single crystal

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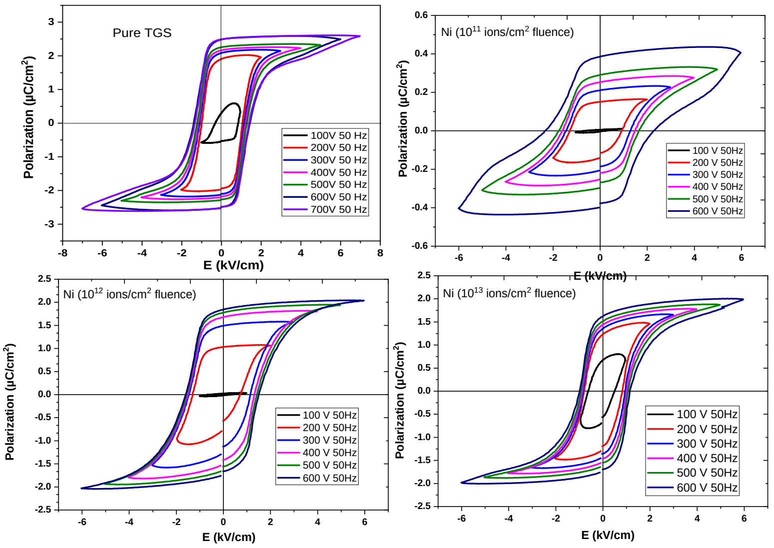
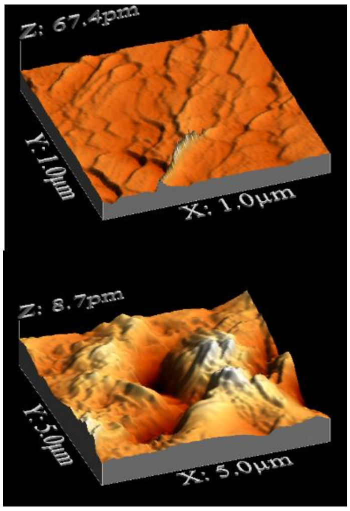
An attempt on the effect of Swift Heavy Ions (SHI) Ni+ (100 MeV) irradiated on the <011> oriented TGS single crystals has been studied. The ion irradiation has been performed at various ion fluencies in order to see the ion matter interaction [1-3] and their consequences in the physical properties of the materials. The optical absorption properties of irradiated crystals ass shifted to a lower band gaps which indicates the presence of defect density states occur nearby to the band edge of TGS materials. A reasonable changes observed in the loop of P-E loops which is due to the change in the internal domain polarization due to the contribution of the implanted nickel ions and the transition temperature has been shifted to 58℃. The surface changes could also have been witnessed from AFM measurements. The overall results obtained have been correlated with proper scientific interpretation.





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P39. Influence of tungsten RDE rotation on the morphology of anodic WO_x formed in NH_4NO_3-based electrolyte

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Nanostructured tungsten oxide is a promising material for photocatalytic air and water purification, photoelectrochemical water splitting, photosensors, electrochromic displays and photonic crystals. WO_x is a deserving candidate for such applications due to its relatively narrow band-gap ~2,6 eV, which makes it sensitive to the visible light, and its relative physicochemical stability in aggressive environments. Nanostructured WO_x has a much higher effective surface area that affords to increase the efficiency of WO_x applications.

Anodization is one of the efficient methods for barrier or nanostructured oxides formation. A lot of regimes of nanostructured WO_x synthesis have been discussed, and anodic WO_x with different morphology (nanoholes, nanobowls, nanowires) has been shown [1, 2, 3]. However, most of the papers evaluate the influence of electrolyte content or anodization current or potential under not well defined hydrodynamic conditions such as magnetic stirring. However, for other oxides, it was shown that hydrodynamic conditions play a crucial role in the kinetics of nanostructured oxide formation and can determine its morphology [4].

In the present study, we investigated the influence of hydrodynamic conditions on the growth of nanostructured anodic WO_x via the Rotating Disk Electrode (RDE) system. The tungsten foils oxidation was performed under different rotation velocities (0 – 1500 rpm).

The morphology of nanostructured WO_x layers was investigated by field-emission scanning electron microscope (FESEM) Helios NanoLab 650. It was found that the morphology could change from almost dense films to the porous films with the pores of around 100 nm in diameter by varying the rotation velocity.

Finally, the photocatalytic degradation of methylene blue (MB) with obtained WO_x photocatalysts. The photoelectrochemical (PEC) properties were studied using a three-electrode system with quartz cell filled with 0.5 M Na_2CO_3.

Acknowledgments

This work was supported by the RFBR, grant 18-29-23038 mk.

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P40. Influence of thermal treatment parameters on functional properties of multi-walled TiO$_2$ NTs

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Anodic titania nanotubes (TiO$_2$ NTs) are widely known as chemical stable photoelectrodes with a high surface area1. Such structures are being intensively investigated for photovoltaic and photocatalytic applications. However, due to the wide bandgap (~3.2 eV) TiO$_2$ is photoactive only under the ultraviolet range of wavelengths (<400 nm) [1]. Such limitation decreases its potential efficiency for photocatalytic applications. Common approaches to increase the photoactivity of TiO$_2$ NTs is the introduction of impurity atoms of metals and nonmetals into its crystal lattice during anodization and post thermal treatments in various atmospheres [2]. It is already known, that the use of electrolytes based on ethylene glycol leads to the incorporation of carbon into the oxide [3]. Carbon modification of TiO$_2$ NTs leads to increase of the absorbance spectra and decrease of the electrical resistance. Previously, the morphology, composition, local distribution of chemical elements, as well as the local phase composition of TiO$_2$ NTs after thermal treatments in air, vacuum and sequential annealing processed in vacuum and air (combine thermal treatment) were investigated [4].

Here we show a comparative analysis of obtained TiO$_2$ NTs with different morphology, chemical and phase composition and their optical, photoelectrochemical and photocatalytic properties.

Technological parameters for the TiO$_2$ NTs based structures were selected for the optimal photocatalytical performance.

Acknowledgments

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P41. Electrochemical properties of electrodes based on anodic TiO_2 nanotubular layers for Al-ion batteries

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At the present, renewable energy devices, especially lithium-ion batteries are widely used in portable electronic devices, including cell phones, laptops, and handheld devices. However, the limited lithium resources and uneven distribution on the ground are the inevitable problems that will prevent the development of lithium-ion batteries for large-scale applications.

Batteries based on Al-ion intercalation have emerged as a potential alternative to lithium-ion batteries [1]. The advantages of such batteries are abundant supplies of aluminum, low cost and safety. The search and study of suitable electrode materials are one of the main tasks in the development of such ionic batteries.

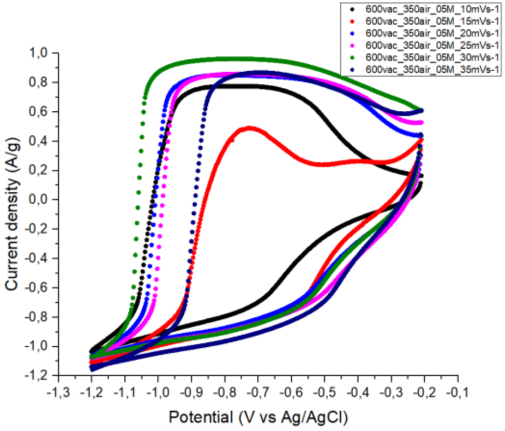

Fig. 1. CV curves of TiO_2-NTA after two-staged thermal treatment, at first in a vacuum at 600°C, then in air 350°C for 1 hour

Titanium oxide (TiO_2) is considered as the one of the most promising electrode materials due to its chemical stability, a large reserve of resources and environmental friendliness [2]. However, pure TiO_2, usually exhibits low electronic and ionic conductivity.

Here we demonstrate a change in the electrochemical properties of an electrode based on an anodic nanotubular titanium oxide layer (TiO_2-NTA) depending on the thermal treatment and electrolyte concentration. The TiO_2-NTAs were obtained by the two-stage anodic oxidation method in a EG-based fluorine-containing electrolyte and then annealed in different atmospheres and at different temperatures. TiO_2-NTA-based electrodes were polarized at 1 mol/L and 0.5 mol /L $AlCl_3$ at cycling rates of 10, 15, 20, 25, 30 mVs^{-1}. The cyclic voltammetry (CV) curves are shown in Fig.1.

Acknowledgments

This work was supported by RFBR grant № 19-33-90287

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P42. Effect of adsorption of epoxide and hydroxyl group on a monolayer graphene sheet: A DFT investigation

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The young's modulus of single layer graphene sheet under uniaxial strain is calculated by applying strain in 3 different configurations (isotropic strain, along zigzag direction and along armchair direction). The obtained value of the young's modulus is comparable to the experimental values. Further, 10 different configuration of monolayer graphene sheet in its functionalized form (GO) with epoxide and hydroxyl group is considered for adsorption studies. The results are discussed and analyzed. The calculations were carried out within the density functional theory (DFT) framework using Quantum ESPRESSO (QE) package [1]. All electronic calculation is done using generalized gradient approximation (GGA) exchange-correlation functional. Electron-ion interaction was treated with pseudopotential method. After testing for convergence of various parameters, the kinetic energy cut-off was set to 50. The integration over the brillouin zone (BZ) was performed employing 18 x 18 x 1 Monkhorst–Pack (MP) k-points mesh for pristine configuration. The atoms in the structure were fully relaxed to till all forces became smaller than $10^{-3}\ eV/\text{Å}$. The energy convergence parameter was set to $10^{-8}\ eV$. For physisorption studies calculation were done using rVV10 density functional for treating non local interaction between graphene layer and adsorbed molecule. The binding energy of the epoxide and hydroxyl functional groups on graphene is calculated with respect to the sum of energies of pristine graphene and isolated O and OH in vacuum as

$$E_b = -(E_{GO} - E_G - nE_O - mE_{OH}) \qquad (1)$$

Similar calculation for binding energy is done for absoption of gases on graphene and GO surface. The optimised structure is used for mechanical strenght investigation. The axial strains were calculated in three different configuration of strain

strain which modifies xy plane isotropically, XY
$$\varepsilon_B = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (2)$$

compression or dialation, modification along zigzag, X,
$$\varepsilon_C = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (3)$$

compression or dialation, modification along armchair, Y,
$$\varepsilon_D = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \varepsilon_{11} & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad (4)$$

The corresponding potential energy is calculated for the strain $\varepsilon = \Delta L/L$ in the range of -0.05 to +0.05 for each case. The potential energy curve was found to have parabolic nature as shown in figure 1. The young's modulus is calculated using expression $Y = \frac{1}{V_O}\frac{\partial E^2}{\partial^2 \varepsilon}$, where V_o is volume of graphene sheet ($V_O = length \times width \times thickness$), for the present case thickness is considered as optimized vander wall distance between each layer of graphene sheet (0.7363 nm). Various configuration for GO structure were initially optimized with varying concentration of epoxide and hydroxyl group as shown in figure 2. The binding energy were calculated using equation 1 and listed in Table 1.

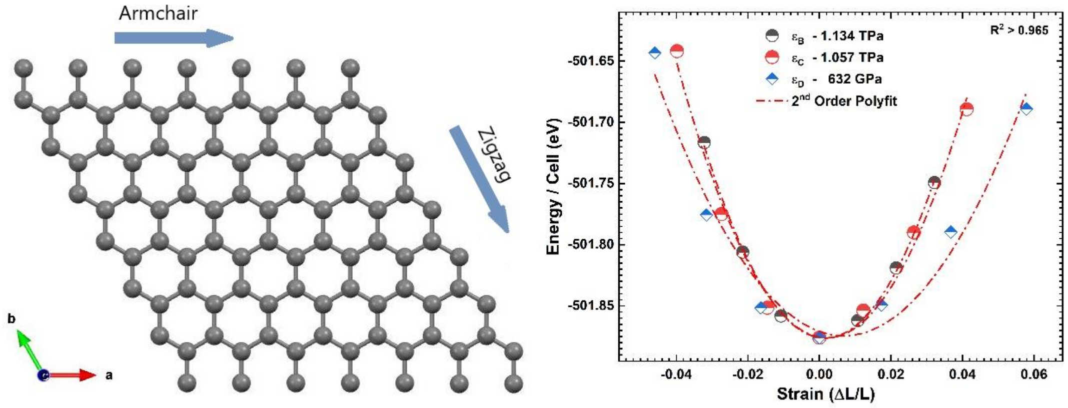

Figure 1. (a) Model of graphene sheet for calculation of mechanical property and (b) potential energy against strain for graphene sheet using DFT.

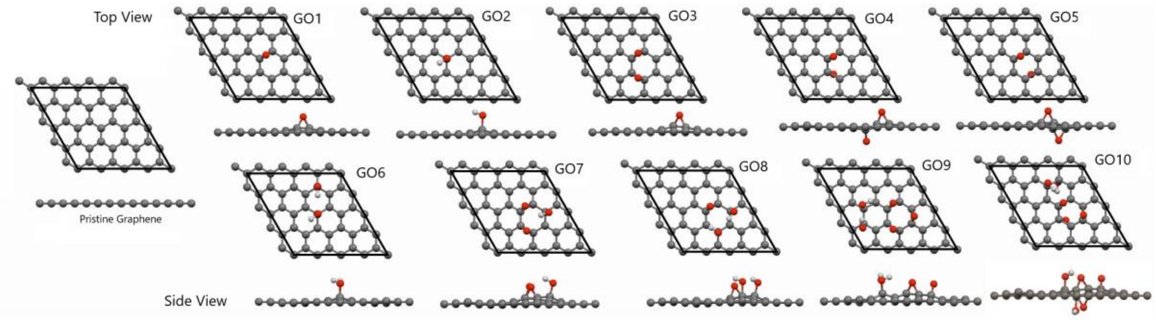

Figure 2. Optimized geometry of various configuration of Graphene Oxide for adsorption study.

Index		Number of elements		Number of sp2 Carbon	Binding Energy (eV)	Eb / O
	Energy (index) (Rydberg)	OH	O			
Gra0	-590.238407	0	0	32	0.0000	0.0000
Gra1	-631.677704	0	1	30	3.8588	3.8588
Gra2	-632.893991	1	0	31	0.8227	0.8227
Gra3	-673.159033	0	2	28	8.2895	4.1447
Gra4	-673.165305	0	2	28	8.3748	4.1874
Gra5	-673.069013	0	2	28	7.0647	3.5323
Gra6	-675.688534	2	0	30	3.5360	1.7680
Gra7	-715.855328	1	2	27	9.6660	3.2220
Gra8	-717.058256	2	1	28	6.4482	2.1494
Gra9	-800.024643	2	3	24	15.3603	3.0721
Gra10	-800.099466	2	3	24	16.3783	3.2757

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Title
3rd International Conference on
Nanomaterials Science and Mechanical Engineering
Book of Abstracts

Editors
Igor Bdikin, Raul Simões

Publisher
UA Editora
Universidade de Aveiro
1st edition – July 2020

ISBN
978-972-789-644-8

university of aveiro tema centre for mechanical technology and automation