International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal
July 16-18, 2018

tema
university of aveiro
centre for mechanical technology and automation

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Book of Abstracts

Editors
Igor Bdikin
Victor Fernando Santos Neto

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The conference (International Conference on Nanomaterials Science and Mechanical Engineering, University of Aveiro, Portugal, July 16-18, 2018) 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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Department of Mechanical Engineering of University of Aveiro

The Department of Mechanical Engineering (DEM) is the unit of University of Aveiro focused on teaching, research and services for the community on the field of Mechanical Engineering.

Prof. Dr. José Grácio (1959-2014), first director of DEM

DEM is responsible for teaching undergraduate and graduate studies in the field of Mechanical Engineering: Integrated Master in Mechanical Engineering (1st and 2nd cycle studies) and Doctoral Program in Mechanical Engineering) (3rd. cycle studies). DEM also shares responsibility for teaching graduate studies in related fields with Mechanical Engineering, including MSc. in Industrial Automation Engineering (2nd cycle studies), MSc. in Product Engineering and Design (2nd cycle studies), MSc. in Sustainable Energy Systems (2nd cycle studies), PhD in Energy Systems and Climate Changes (3rd cycle studies) and PhD in Nanosciences and Nanotechnologies (3rd cycle studies). All the studies cycles are organized following the Bologna process. The graduates in Mechanical Engineering by the University of Aveiro are very well accepted, and highly wanted, by the labor market, both at the Nacional and International levels. Graduates from the UA have achieved, in a short period, positions of leadership and responsibility in organizations and companies where they develop their professional activity.

Research and development are mainly conducted under the DEM Research Unit, the Centre for Mechanical Technology and Automation (TEMA). It is TEMA that gives to DEM an institutional profile where scientific research plays an important role. The main areas of activity include as main pillars: Automation, Thermal Fluid Sciences, Mechanical Technology, Mechanical Design, Applied and Computational Mechanics, and Nanoengineering. Other relevant areas of activity include Product Development, Biomechanics, Energy, and Nanosciences and Nanotechnologies. Connections between the different pillars and areas of activity are strongly encouraged.

DEM has a true university profile, with a prestigious faculty that has done much and will continue to do for teaching, research and cooperation with society.

We would welcome interested visitors to come and see our new facilities and learn more about mechanical engineering. For additional information about DEM: http://www.ua.pt/dem/

Welcome to the Department of Mechanical Engineering of the University of Aveiro!

Professor Dr. Vítor António Ferreira da Costa
Director - Department of Mechanical Engineering
University of Aveiro
Campus Universitário de Santiago
3810-193 AVEIRO
PORTUGAL

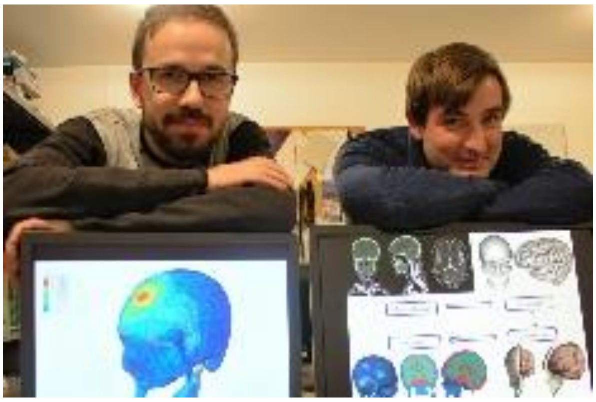
Centre for Mechanical Technology Automation (TEMA), Department of Mechanical Engineering, University of Aveiro

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

Grounded on its human capital and their competences, TEMA is focused on relevant societal challenges aiming to contribute to a sustainable industry (specially SMEs) and to the wellbeing of people, translated into two main future mobilizing projects: Sustainable Manufacturing Solutions and Technologies for the Wellbeing.

A group of students from the University of Aveiro (under supervision of João Oliveira, a professor at the Department of Mechanical Engineering) has just created Aquila, a single-seat car based on the Formula One style, which aims to compete in the Silverstone circuit during the Formula Student challange.

Sustainable Manufacturing Solutions is focused on the development and innovation of manufacturing engineering and technologies, with subsequent industrial applications. It is intended to increase productivity, improve products quality and reduce waste in production processes. The strategy on Technologies for the Wellbeing aims to increase the quality of life of society by means of engineering systems, focusing on people and their needs.



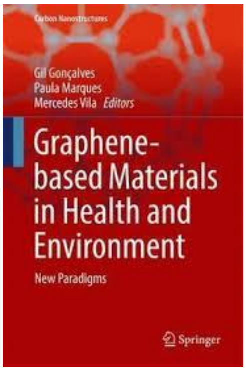
Prof. Dr. Ricardo José Alves de Sousa and Dr. Fábio Fernandes

Through computer numerical simulation, a group of researchers from the University of Aveiro (UA) created a system capable of simulating the impact of an object when it collides with the human head and assesses which lesions (and how severely) can reach the victim. Designed to test the effectiveness of a new generation of cork-lined helmets, the design can also be applied in forensic medicine at the time, for example, for the reconstruction of accidents.

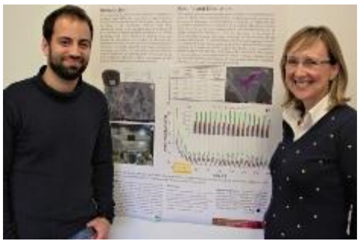
TEMA has been contributing to solve several challenges by means of high-level research and development on: (i) new products based on both traditional and nanoengineering technologies; (ii) computational and experimental tools to enhance quality, minimize costs, reduce raw materials and energy requirements; and (iii) new and optimized technologies for increased effectiveness in terms of energy requirements and production schedules.

A group of students from the University of Aveiro (under supervision of António Bastos, a professor at the Department of Mechanical Engineering) participates actively in the conception of prototype racing motorcycles based on the Moto3 category, to participate in the International MotoStudent Competition that is held in the Aragón Motorland track every two years. It is now in the end of the manufacturing process of its second participation.

TEMA researchers form one coherent group with competences in the fields of applied mechanics, modelling and simulation, nanoengineering, biomechanics, transportation technologies, applied energy, together with transdisciplinary areas aligned to the priorities of the international agenda towards equality, gender balance, diversity, and scientific and technological excellence.



Researcher at the Department of Mechanical Engineering (DEM) of the University of Aveiro (UA), the work of André Girão aims at the preparation of new three-dimensional biomaterials based on graphene oxide and collagen for tissue engineering applications.



The award-winning paper is part of the project "An integrated approach using stimulus responsive 3D graphene / collagen scaffold for tissue engineering" by researcher Paula Marques of TEMA, entitled "Graphene oxide-collagen scaffold as a versatile microenvironment for mechanical stimulation on tissue engineering".

TEMA researchers have already contributed to these fields in the past 5 years, with 864 published papers in international peer-reviewed journals. Between 2013 and 2017, TEMA supported the training of more than 340 Master and 50 PhD students, who successfully concluded their studies. National and International keynote lectures were delivered in the areas of computational mechanics, biomechanics, plastic forming, nanotechnology, transportation systems and applied energy.

Prof. Dr. Vítor Manuel Ferreira dos Santos and master's student Nuno Santos. Department of Mechanical Engineering of the UA and Robotics Group of the Institute of Electronic Engineering and Telematics of Aveiro (IEETA). studies robots that choose and classify pieces placed at random.

TEMA is therefore prepared to properly address and promote scientific and technological projects of medium to high complexity, with multidisciplinary characteristics. Collaboration with national and international industrial agents currently represent almost 50% of the overall research activities, being TEMA part of the Portuguese Roadmap of Research Infrastructures, as well as of the European Union Map of Institutions strategic for the development of Key Enabling Technologies (KET).

Currently, the management structure of TEMA is composed by the Board of Directors (a director and five deputy directors), the Scientific Council, the External Scientific and Industrial Advisory Board, and the General Assembly. Based on the expertise of TEMA members, until 2017 the organization relied on 6 research groups, each one led by a coordinator for the research activities within the group and the articulation between the strategy of each group and the research unit. The Scientific Council is composed by all effective members, with a deliberative role. The External Scientific and Industrial Advisory Board is made of five external reputed academic and industrial personalities, responsible for real time assessment of TEMA activities, counseling and monitoring of the alignment between those activities and the research unit's mission.

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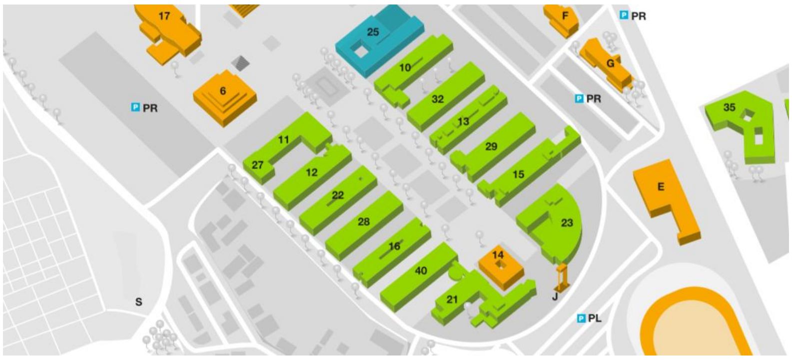
SCIENTIFIC PROGRAM

University Aveiro, Complexo Pedagógico (auditorium 23.1.5) 16.07-18.07. 2018



MONDAY, JULY 16, 2018	
9:00 - 12:00	**REGISTRATIONS**
9:30 - 10:00	**WELCOME ADDRESS:** **Prof. Dr. Vítor António Ferreira da Costa** **Prof. Dr. António Manuel de Bastos Pereira** **Dr. Paula Alexandrina de Aguiar Pereira Marques** **Dr. Duncan Paul Fagg** **Dr. Igor Bdikin** **Prof. Dr. Victor Fernando Santos Neto**
	Session: Nanocomposite films **CHAIRS: Victor Fernando Santos Neto**
10:00 - 11:00	**PLENARY LECTURE: Vincent BALL** ***Université de Strasbourg, France*** ***Institut National de la Santé et de la Recherche Médicale, Strasbourg Cedex, France*** **Title: Catechol and polyphenol based composite coatings: a versatile method to confer functionality and mechanical properties at interfaces.**
11:00 - 11:30	**COFFEE BREAK/POSTER SESSIONS**
	Session: Nanocomposite films and surface properties in Nano and Micro level **CHAIRS: Victor Fernando Santos Neto**
11:30 - 12:00	**LECTURE: Fábio Gabriel Nazário Figueiras** ***CICECO-Aveiro Institute of Materials, Department of Ceramics and Glass Engineering, University of Aveiro, Aveiro, Portugal*** ***IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física da Faculdade de Ciências da Universidade do Porto, Portugal*** **Title: Thriving Narrow Band Gap Ferroelectric Oxides for Photovoltaic Applications: Bi_2ZnTiO_6 Thin Films Deposited by RF Sputtering.**

12:00-13:00	**LECTURE: Ezddin Hutli,** *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 **Title: Cavitation as tool to modify and enhance materials surface properties in Nano and Micro level.**
13:00 – 14:00	**LUNCH BREAK**
	Session: Nanomaterial/nanocomposite properties and applications **CHAIRS: Gonzalo Guillermo Otero Irurueta**
14:00 - 15:00	**PLENARY LECTURE: Nikolai Sobolev** ***Department of Physics and I3N, University of Aveiro, Portugal*** **Title: Ion irradiation in the technology of perpendicular magnetic tunnel junctions.**
15:00 - 15:30	**LECTURE: Svitlana Kopyl** ***Department of Physics & CICECO-Aveiro Institute of Materials, University of Aveiro, Portugal*** **Title: Diphenylalanine peptide nanotubes with different chirality: structures, properties, and applications.**
15:30 - 16:00	**LECTURE: Pukazh Selvan Dharmakkon** ***Researchers Centre for Mechanical Technology Automation (TEMA), Mechanical Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal*** **Title: Exploring the catalytic reaction mechanism of metal oxide additives loaded hydrogen storage system MgH_2.**
16:00- 16:30	**COFFEE BREAK/POSTER SESSIONS**
	Session: Nanomaterial/nanocomposite properties and applications **CHAIRS: Nikolai Sobolev**
16:30 - 17:30	**PLENARY LECTURE: José Maria da Fonte Ferreira** ***Department of Materials and Ceramics Engineering, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal*** **Title: The big challenges of small scale fabrication of functional lead free piezoelectric ceramics.**
17:30 - 18:00	**LECTURE: Denis Alikin** ***School of Natural Science and Mathematics, Ural Federal University, Ekaterinburg, Russia*** ***Department of Physics & CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal*** **Title: Nanoscale studies of ionic conductor materials by strain-based scanning probe microscopy.**

TUESDAY, JULY 17, 2018	
	Session: 2D nanomaterials **CHAIRS: Paula Marques and Teresa Portolés**
9:00 - 9:30	**LECTURE: María Teresa Portolés** ***Departamento de Bioquímica y Biología Molecular, Facultad de Ciencias Químicas, Universidad Complutense de Madrid (UCM), Madrid, Spain*** **Title: In vitro models for evaluating specific cell responses to graphene oxide and other nanoparticles.**
9:30 - 10:00	**LECTURE: Gil Goncalves** ***Instituto de Ciencia de Materiales de Barcelona (ICMAB-CSIC), Bellaterra, Spain*** **Title: Graphene oxide: a basic unit for the controlled self-assembly of 3D carbon macrostructures by supercritical CO_2.**
10:00 - 10:30	**LECTURE: María Concepción Serrano López-Terradas** ***Instituto de Ciencia de Materiales de Madrid (ICMM), Consejo Superior de Investigaciones Científicas (CSIC), Madrid, Spain*** **Title: Reduced graphene oxide-based materials for neural regeneration at the injured spinal cord.**
10:30 - 11:00	**COFFEE BREAK/POSTER SESSIONS**
	Session: 2D nanomaterials **CHAIRS: Paula Marques and Ermelinda Maçoas**
11:00 - 12:00	**PLENARY LECTURE: Nuno Miguel Machado Reis Peres** ***University of Minho, Physics Department, Braga, Portugal*** **Title: Plasmonics with graphene.**
12:00 - 12:30	**LECTURE: Cristina Freire** ***REQUIMTE/LAQV, Departamento de Química e Bioquímica, Faculdade de Ciências, Universidade do Porto, Porto, Portugal*** **Title: Graphene nanocomposites in chemical catalysis and energy-related electrocatalysis.**
12:30 - 13:00	**LECTURE: Ermelinda Maçôas** ***Centro de Química-Física Molecular e Centro de Química Estrutural do Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal*** **Title: Selective Two-Photon Absorption in Carbon Dots: an extra piece of the puzzle of photoluminescence emission.**
13:00 - 14:00	**LUNCH BREAK**

	Session: Modeling of nano- and micromaterials **CHAIRS: Igor Bdikin**
14:00 - 15:00	**PLENARY LECTURE: Vladimir Bystrov** ***Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*** **Title: Modeling of polymer ferroelectrics/graphene nano-composites.**
15:00 - 15:30	**LECTURE: Anuraag Gaddam** ***Department of Materials and Ceramic Engineering, CICECO, University of Aveiro, Portugal*** **Title: Statistical mechanical modeling of the glass structure.**
	Session: Mechanical Engineering Optimization (Theory and Applications) **CHAIRS: António Manuel de Bastos Pereira and António Carlos Mendes de Sousa**
15:30 - 16:00	**LECTURE: Kiryl Yasakau** ***Department of Materials and Ceramic Engineering/CICECO–Aveiro Institute of Materials, University of Aveiro, Portugal*** **Title: Reflections on localized corrosion of metallic alloys and corrosion protection strategies.**
16:00 - 16:30	**COFFEE BREAK/POSTER SESSIONS**
	Session: Mechanical Engineering Optimization (Theory and Applications) **CHAIRS: António Manuel de Bastos Pereira and António Carlos Mendes de Sousa**
16:30 - 17:00	**Oral presentation: Ezddin Hutli,** Milos Nedeljkovic, Attila Bonyár, ***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** **Statistical Analysis of Variation of Cavitation Cloud characteristics in Space and Time and Related Behavior Based on the Flow Condition.**
17:00 - 17:30	**LECTURE: Alexey Sherchenkov** ***National Research University of Electronic Technology, Moscow, Russia*** **Title: Mechanical properties and adhesion of the thin films of phase change memory materials.**

	Session: PhD student SHORT COMMUNICATIONs **CHAIRS: Igor Bdikin**
17:30 - 17:45	**SHORT COMMUNICATION: Magdalena Wypij** ***Department of Microbiology, Faculty of Biology and Protect Environment, Nicolaus Copernicus University, Toruń, Poland*** **Title: Synthesis and antimicrobial and cytotoxic activities of silver nanoparticles synthesized from Streptomyces palmae OF1 strain.**
17:45 - 18:00	**SHORT COMMUNICATION: Marta Pakiet** ***Adam Mickiewicz University in Poznan, Faculty of Chemistry, Laboratory of Microbiocides Chemistry, Poznań, Poland*** **Title: Efficiency of cationic surfactants with polyamine platform as corrosion inhibitors of stainless steel and carbon steel.**
19:00 - 20:30	**Banquet**

WEDNESDAY, JULY 18, 2018	
	Session: Nanoscale measurements of materials **CHAIRS: Igor Bdikin**
9:00-9:30	**LECTURE: Sergey Bozhko** ***Institute of Solid State Physics, Russian Academy of Science, Chernogolovka, Moscow District, Russia*** **Title: Scanning tunneling microscopy of surface states in topological insulators.**
9:30-10:30	**PLENARY LECTURE: Senentxu Lanceros-Méndez** ***BCMaterials, Parque Científico y Tecnológico de Bizkaia, Derio, Spain IKERBASQUE, Basque Foundation for Science, Bilbao, Spain*** **Title: Nanoengineering of organic materials for smart and multifunctional application.**
10:30- 11:00	**COFFEE BREAK**
	Session: 2D nanomaterials **CHAIRS: António Manuel de Bastos Pereira, Igor Bdikin**
11:00-12:00	**PLENARY LECTURE: Pedro Alpuim** ***International Iberian Nanotechnology Laboratory, Braga, Portugal*** **Title: Biosensing with graphene.**
12:00-12-30	**Oral presentation: Abdelkadir Belhadj,** Abdelkrim Boukhalfa, Sid A Belalia, *Computational Mechanics Laboratory, Department of Mechanical Engineering, Faculty of Technology, University of Tlemcen, Tlemcen, Algeria* **On the vibration behavior of rotating nanostructures.**
12:30-12:45	**Oral presentation: Ana R. Monteiro,** Catarina I. V. Ramos, Sara Fateixa, Nuno M. M. Moura, Maria G. P. M. S. Neves, Tito Trindade**,** *QOPNA and CICECO-Aveiro Institute of Materials, Department of Chemistry of University of Aveiro, 3810-193 Aveiro (Portugal)* **Porphyrin@GO hybrid materials as DNA G-quadruplex detectors and stabilizers.**
12:45 – 13:00	**Finish and Finishing remarks**
13:00 – 14:00	**LUNCH BREAK**
14:00-18:00	**DEM, NRD lab. Excursions**

POSTERS

P1	V.S. Bystrov, Budhendra Singh, I.K. Bdikin, V.A. Tverdislov, O.A.Zhulyabina, *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia; TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, 3810-193 Aveiro, Portugal. Physical Faculty, Lomonosov Moscow State University, Moscow, Russia* **Ferroelectric physical properties of various dipeptide nanotubes**
P2	M. Cicuéndez, J. Santos, A. Coimbra, H. Oliveira, M. Ayán–Varela, J. I. Paredes, S. Villar–Rodil, M. Vila, V.S. Silva, *NRG-TEMA, Mechanical Engineering Department, University of Aveiro (UA). Campus Universitário de Santiago. 3810-193 Aveiro, Portugal. CICECO - Aveiro Institute of Materials, Chemistry Department, University of Aveiro (UA). Campus Universitário de Santiago. 3810-193 Aveiro, Portugal. CESAM & Department of Biology, University of Aveiro. Campus Universitário de Santiago, 3810193 Aveiro, Portugal. Instituto Nacional del Carbón, INCAR-CSIC, Apartado 73, 33080 Oviedo, Spain* **MoS_2 flakes stabilized with DNA/RNA nucleotides: *In vitro* cell response**
P3	Bystrov V.S., Paramonova E.V., Avakyan L.A., Coutinho J., Bystrova A.V. Yu.D. Dekhtyar, *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia. Physics Faculty, Southern Federal University, Rostov-on-Don 344090, Russia. Department of Physics and I3N, University of Aveiro, 3810-193 Aveiro,Portugal. Biomedical Engineering and Nanotechnology Institute, Riga Technical University, Riga, Latvia* **Hydroxyapatite with defects by first-principles calculations**
P4	Magdalena Wypij, Patrycja Golinska, Hanna Dahm. *Department of Microbiology, Faculty of Biology and Protect Environment, Nicolaus Copernicus University, Poland, Gagarina 11 87-100 Torun, Poland* **Synthesis and antimicrobial and cytotoxic activities of silver nanoparticles synthesized from *Streptomyces palmae* OF1 strain**
P5	M.V. Silibin, V.S. Bystrov, D.A. Kiselev, Pegah Mirzadeh, P.A.A.P. Marques, B.Singh, I.K. Bdikin, *National Research University of Electronic Technology, Zelenograd, Moscow, Russia. Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia. National University of Science and Technology "MISiS", Moscow, Russia. TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **Local piezoelectrical properties of P(VDF-TrFE)/ Graphene and P(VDF-TrFE)/ Graphene oxide composite fibers**
P6	Marta Pakiet, Iwona Kowalczyk, Rafael Leiva Garcia, Robert Akid, Bogumil Brycki, *Adam Mickiewicz University in Poznan, Faculty of Chemistry, Laboratory of Microbiocides Chemistry, Umultowska 89b, 61-614 Poznań, Poland. School of Materials, University of Manchester, Manchester, M139PL, UK* **Efficiency of cationic surfactants with polyamine platform as corrosion inhibitors of stainless steel and carbon steel**
P7	Bruno Miguel da Silva Teixeira, *Physics Department and i3N, University of Aveiro, Portugal* **Double MgO/FeCoB interface free-layer for perpendicular magnetic tunnel junctions: effect of thickness and metallic spacer**

P8	**Sergei Dubkov,** Dmitry Karpinsky, Vladimir Khomchenko, Maxim Silibin, *National Research University of Electronic Technology, Shokina Square, Building 1, Zelenograd, Moscow, Russia, Russia. Scientific-Practical Materials Research Centre of NAS of Belarus, Minsk, Belarus. CFisUC, Department of Physics, University of Coimbra, P-3004-516 Coimbra, Portugal* **Improved functional properties of co-doped $BiFeO_3$ compounds**
P9	**Maxim Silibin,** *National Research University of Electronic Technology, Moscow, Russia* **Preparation, stability and local physical properties of P(VDF-TrFE)/Graphene oxide composite thin films and nanofibers**
P10	**Ângela Semitela,** Carla Fernandes, André F. Girão, António Completo and Paula A.A.P. Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **Improving surface properties and porosity of electrospun scaffolds for cartilage tissue engineering**
P11	**Carla Fernandes,** Ângela Semitela, António Completo and Paula A.A.P. Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **Cell seeding process optimization on polycaprolactone-gelatin-arcade-like-architecture-scaffolds**
P12	**André F. Girão,** Joana Sousa, María C. Serrano, António Completo and Paula A.A.P. Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **A biomimetic tissue engineering scaffold for repairing the injured spinal cord: proof of concept**
P13	**Joana Sousa,** André F. Girão, Sandra Vieira and Paula A.A.P. Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **Polycaprolactone-gelatin-graphene oxide electrospun nanofibers for tissue engineering applications**
P14	**Sahil Goel**, Nidhi Sinha, Budhendra Singh, Igor Bdikin and Binay Kumar, *Crystal Lab, Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India, Department ofElectronics, SGTB Khalsa College, University of Delhi, Delhi 110007, India, TEMA-NRD, MechanicalEngineering Department, Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro 3810-193, Portugal,* **8-hydroxyquinolinium hydrogen squarate crystal: a new piezoelectric and NLO active crystal**
P15	**Abhilash J. Joseph, Nidhi Sinha, Abid Hussain, Sahil Goel, Budhendra Singh, Igor Bdikin, Binay Kumar,** *Crystal Lab, Department of Physics and Astrophysics, University of Delhi, Delhi 110007, India, Department ofElectronics, SGTB Khalsa College, University of Delhi, Delhi 110007, India, TEMA-NRD, Mechanical Engineering Department, Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro 3810-193, Portugal* **Crystal growth and characterizations of flux grown MPB compositions of ferroelectric PZN-PT and PMN-PT single crystals**

P16	**Igor Bdikin,** Budhendra Singh, V.S. Bystrov, *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* **Local piezoelectricity in amino acids microcrystals**
P17	**Susana C. Pinto,** Ricardo Pinto, Isabel Duarte, Romeu Vicente, Carmen Freire and Paula A.A.P. Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **Multifunctional aerogels by combining nanocellulose and graphene based materials**
P18	**M.S. Ivanov,** F. Amaral, V.A. Khomchenko, and L.C. Costa and J.A. Paixão, *CFisUC, Department of Physics, University of Coimbra, Portugal; College of Health Technology of Coimbra, Polytechnic Institute of Coimbra, Portugal; I3N & Physics Department, University of Aveiro, Portugal* **Discovery of the conductivity behaviour of $CaCu_3Ti_4O_{12}$ by using Scanning Probe Microscopy technique**
P19	Smaail Radi, Chahrazad El Abiad, **Nuno M. M. Moura,** Maria A. F. Faustino, M. Graça P. M. S. Neves, *Laboratory of Applied Chemistry and Environment (LCAE), Department of Chemistry, Faculty of Sciences, University Mohamed Premier, Oujda, Morocco; QOPNA and Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal* **Porphyrin-based organic-inorganic hybrid on the removal of metal ions**
P20	**Ana Bessa**, Bruno Henriques, Gil Gonçalves, Maria Eduarda Pereira, Paula Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal, CESAM & Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal* **GRAFENE OXIDE MACROSTRUTURES FOR THE REMOVAL OF HEAVY METALS IN CONTAMINATED WATERS**
P21	**Gonçalo Ramalho,** André F. Girão, Ângela Semitela, António Completo and Paula A.A.P. Marques, *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, Portugal* **Design and fabrication of anisotropic scaffolds towards cartilage tissue engineering**
P22	**João Nogueira**, Tito Trindade, Ana Luísa Daniel da Silva, *CICECO – Aveiro Institute of Materials and Chemistry Department, University of Aveiro, 3810-193 Aveiro, Portugal* **Porous carrageenan-based carbons for water treatment**
P23	**Maxim Shtern**, Maxim Rogachev, Yuri Shtern, Alexey Sherchenkov, Dmitry Gromov, Alexander Kozlov, *National Research University of Electronic Technology (MIET), Moscow, Russia* **Development of the contact system for the effective multisectional thermoelements with the operating temperature range from 300 to 1200 K**
P24	**Francisco Lopes, Ana Horovistiz, António Completo, J. Paulo Davim,** *TEMA, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal* **Morphological characterization of surfaces manufactured by High-speed machining: Fractal approach of surface topography of tibial insert in UHMWPE**

P25	**D. Machado**, M. J. Hortigüela, R. Silva, P.A.A.P. Marques, Rui Silva, G. Otero-Irurueta, V. Neto, *Centre for Mechanical Technology and Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, 3810-193 AVEIRO, PORTUGAL. Aveiro Institute of Materials (CICECO), Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 AVEIRO, PORTUGAL* **Graphene based sensors for air quality monitoring**
P26	**M. J. Hortigüela**, D. Machado, I. Bdikin, V. Neto and G. Otero-Irurueta, *Centre for Mechanical Technology and Automation (TEMA), Department of Mechanical Engineering, University of Aveiro, 3810-193 AVEIRO, PORTUGAL. Aveiro Institute of Materials (CICECO), Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 AVEIRO, PORTUGAL* **Graphene/MoS_2 vertical heterostructures**
P27	**A. Durairajan,** E.Venkata Ramana, M.P.F.Graça, M.A. Valente, *I3N-Aveiro, Department of Physics, University of Aveiro, Aveiro 3810 193, Portugal* **Exploring Temperature Dependent Raman and Magnetization in ErFeO3 Single Crystal**
P28	V.C. Bharath Sabarish, A.Durairajan, E. V. Ramana, M. A. Valente, I. Bdikin, **G. Ramesh Kumar,** *Departement of Physics, University College of Engineering Arni -Thatchur 632 326, India. I3N-Aveiro, Department of Physics, University of Aveiro, Aveiro 3810 193, Portugal. Department of Mechanical Engineering & TEMA- Centre for Mechanical Technology and Automation, University of Aveiro, 3810-193 Aveiro, Portugal* **Gamma Irradiation Induced Effect on Ferroelectric Triglycine Sulphate (TGS) Single Crystals**

Plenary Lectures

Modeling of polymer ferroelectrics/graphene nano-composites

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The recent achievements in the field of computer modelling as well comparison with the experimental studies of new nano-composite materials based on the polymer ferroelectrics and graphene/oxide graphene are presented in this review lecture. The main results of the computer molecular modelling of the various nanostructures, its physical properties, such as, the polarization changes and polarization switching, piezoelectric and pyroelectric properties of such nanocomposites constructed from thin films of polyvinylidene fluoride (PVDF)/poly(vinylidene fluoride-trifluoroethylene) (P(VDF-TrFE)) and graphene/graphene oxide (G/GO) were calculated and analyzed in comparison with various known experimental data at the nanoscale, in particular, with the data of atomic force and piezo-response force microscopy (AFM/ PFM). Polymer ferroelectric thin and ultra-thin two-dimensional high-ordered films were created firstly by Langmuir-Blodgett (LB) technique [1,2]. It is good object for computer modeling [3].

Polarization switching in PVDF/P(VDF-TrFE) Langmuir-Blodgett (LB) thin films using molecular dynamic (MD) simulation method with the quantum-mechanical (QM) calculations on each step of the MD run was studied [4,5]. For this purpose the semi-empirical PM3 approximation from Hyperchem software package was used. Simulations showed that the polarization switching for ultra-thin films proceeded corresponding to the intrinsic homogeneous switching mechanism in accordance with the theory of Landau-Ginzburg-Devonshire (LGD). Values of coercive field are within 0.5–2.5 GV/m, which is consistent with experimental data. At high values of applied electric field and for thick LB samples the polarization switching corresponds to the Kolmogorov-Avrami-Ishibashi domain mechanism. Critical width begins from (3–6) nm being in line with experimental 10 nm. These data describe the polarization switching for transition from homogeneous to inhomogeneous region for ultrathin polymer ferroelectrics. Analysis shows that for ultrathin PVDF film the dielectric permittivity must have $\varepsilon \sim 2.4$, while for usual bulk one $\varepsilon \sim 5–10$. So, it is lowering when PVDF film thickness decreasing upto 1-2 monolayer.

To clarify the possible mechanism of the domain formation in transition region we performed the density functional theory calculations in local density approximations in AIMPRO codes using orthorhombic unit cell for PVDF model [5]. Computed data show that density of states has energy gap $E_g \sim 6.3$ eV in good comparison with known data.

The computer simulation of the PVDF/P(VDF-TrFE) thin films and polymer-based polymer composite nanostructures of G/GO and PVDF was studied by the different methods using the HyperChem software package: molecular mechanics (MM) (such as, BIO CHARM), quantum mechanics (QM) using semi-empirical PM3 approach, etc.[6-8]. The calculations of the piezoelectric coefficients for all studied structures were performed using the special own developed algorithm [4]. The piezoelectric response, the dielectric constant and the mechanical properties of the films were studied experimentally and found that they depend on the presence of the G/GO content and varied with its concentration. The experimental results correlated qualitatively with the results obtained in the calculations. Calculated data of the piezoelectric coefficients $d_{33} \sim 12$ - 30 pm/C for PVDF-G/GO models corresponding are in line to their observed experimental behavior and variations, when the concentration (composition) of GO components is changed [6-8].

The pyroelectric coefficients for the PVDF and PVDF-graphene structures, were calculated using the MD run with the PM3 quantum method [9]. The calculations of the change in the polarization with increasing temperature were carried out by MD run at the each temperature and P(T) dependence was constructed, which was revealed good agreement with the thermodynamic theoretical dependence obtained from LGD theory. On the basis of this relationship obtained, the pyroelectric coefficients were calculated, which are in line with the known values: in the case of pure PVDF, it is ~ 40 $\mu C/(m^2*K)$. For composite models with graphene it turned out that in the case of a single-layer graphene model the pyro-coefficient is increased by 3-4 times, and for the case of a two-layer model (sandwich model) it is decreased by 2-3 times in comparison with a pure polymeric ferroelectric [9]. To verify and properly evaluate these results, it is necessary to synthesize a thin PVDF/G(GO) film sample of such a composite by using the Langmuir-Blodgett (LB) method, applying PVDF layers to the substrate from graphene layers. Such work is now in progress. Another possible way is based on the fabrication of the spun composites films and the direct measurements of their pyroelectric coefficients.

The obtained results give us the new important information on our understanding of the polarization switching, mechanisms of piezoelectricity and pyroelectricity in these new ferroelectric nanocomposites, give us a new perspective for their further creation, development and applications of such new nanocomposites with the nanoscale polymer-graphene structures as the multi-functional nanomaterials in many fields of nanosciences.

Acknowledgement

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Catechol and polyphenol based composite coatings: a versatile method to confer functionality and mechanical properties at interfaces

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In this presentation, versatile coating methods based on the use of cathecolamines, inspired by the composition of the foot proteins in mussels, and polyphenols, inspired by the deposition of a film from tea or from wine, will be described from structural and mechanistic points of view [1,2]. The ability of those coatings to be postmodified with nanoparticles[3] and molecules containing nucleophiles will then be described. Composite and anisotropic films can be produced at the solid – liquid [4] and the air water interface with remarkable moisture dependent adhesion[5]. Those catecholamine and polyphenol containing films display exceptional optical[6] and mechanical properties[7].

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Ion irradiation in the technology of perpendicular magnetic tunnel junctions

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The magnetic properties of ultrathin magnetic films and multilayers, e.g. magnetic anisotropies and exchange coupling, strongly depend on the surface and interface structure. Chemical composition, crystallinity, grain sizes and their distribution govern the magnetic behaviour. All these structural properties can be modified by particle irradiation. Magnetic patterning without affecting the surface topography becomes feasible, which may be of interest in applications. Homogeneous ion irradiation through masks and focused ion beam and ion projection lithography can be applied for patterning. The creation of magnetic feature sizes down to a few ten nm is possible. The main areas are magnetic data storage applications, such as hard magnetic media with a large perpendicular magnetic anisotropy (PMA) or patterned media with an improved signal-to-noise ratio and magnetic sensor elements.

The PMA is very common at magnetic metal/oxide interfaces. It is thought to be the result of electronic hybridization between the oxygen and the magnetic transition metal orbit across the interface. Interest in this phenomenon appeared in 2010 when it was demonstrated that the PMA at magnetic transition metal/oxide interfaces could be used to build out-of-plane magnetized magnetic tunnel junctions (MTJ) for spin-transfer-torque magnetic random access memory (STT-MRAM) cells. In these systems, the PMA at the CoFeB/MgO interface can be used to simultaneously obtain good memory retention, thanks to the large PMA amplitude, and a low write current, thanks to a relatively weak Gilbert damping.

We'll give a short overview over the irradiation experiments aiming at a modification of magnetic and magnetoresistive properties of different layered magnetic structures. Then we'll describe in detail our recent experiments on ion irradiation of double-MgO free layers designed for application in perpendicular MTJ. The samples comprised a MgO / FeCoB / X / FeCoB / MgO layer stack, where X stands for an ultrathin (0.2 nm) Ta or W spacer. In particular, we have induced easy-cone states, with different cone angles, in thin (t_{FeCoB} = 2.6 nm) free layers with a W spacer, initially exhibiting a uniaxial anisotropy (Figure 1). This easy cone only exists if $K_1 > 0$, $K_2 < 0$ and $– K_2 > 2K_1$, with K_1 and K_2 being the first- and second-order anisotropy constants. Easy-cone anisotropy may help reduce the stochasticity of the spin transfer torque switching. Importantly, no increase in the Gilbert damping after irradiation has been observed.

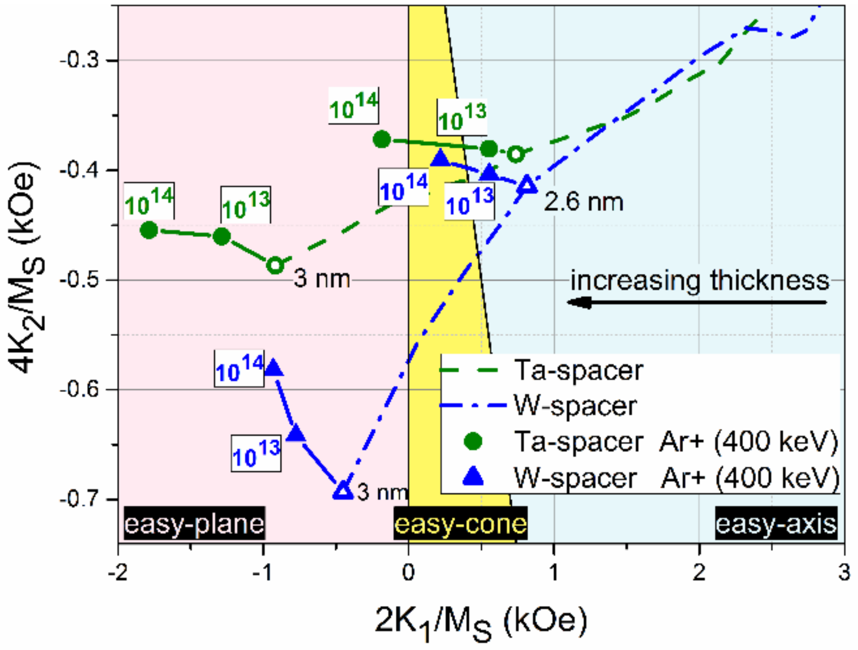

Figure 1. Diagram of implantation-driven transitions between different regimes in free layers with Ta (green dots) and W spacers (blue triangles). Dashed lines and open symbols are the thickness-dependent anisotropy fields prior to implantation.

Biosensing with graphene

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The importance of biosensors in biomedical research is increasing fast, as they are routinely used in a wider range of applications, from prognosis and diagnosis to personalized medicine. Graphene low-dimensionality, high carrier mobility and chemical stability, allow to fabricate relatively simple and highly sensitive biosensors, based on different types of devices. Electrolyte-gated field-effect transistors (EGFETs), where the graphene channel is directly exposed to the analyte, have exceedingly high detection sensitivity, whereas electrochemical microelectrode arrays (EMAs, figure 1) have all the advantages of single microelectrodes (higher current density, faster mass transport and lower detection limits), while providing amplification of the signal by the array.

A preliminary issue that needs to be addressed before graphene devices may be used as biosensors, is to provide them with selectivity for particular targets. In fact, pristine graphene devices will react indistinctly to any charged or polar species placed in their neighborhood. Therefore, functionalization of the graphene surface with molecular probes for biorecognition of desired biomarkers, is necessary (see figure 2). Also, important to keep in mind is that hydrophobic interactions can compromise the particular conformational characteristics of molecules, especially of proteins, and so tailoring the hydrophobicity of pristine graphene for the immobilization of biological species is a critical challenge. Our choice is to modify the graphene surface with a pyrene linker that binds to graphene via π-π interaction and covalently to the probe. In this way, the sp^2 conjugated system of graphene is preserved and with it, the unique electronic properties of the material.

In contrast to the more commonly used chemically modified graphene oxides and graphene flakes, in our work the devices are made of a single layer of chemical vapor deposited graphene. This choice ensures the best possible electronic material, second only to exfoliated graphene from HOPG, while allowing for fabrication at the wafer scale with high precision and reproducibility.

In a standard CVD process, the high density of graphene boundaries will induce carrier scattering, hindering the performance of graphene biosensors. Here, this issue is overcome by growing graphene in a confined graphite space, effectively suppressing Cu sublimation, thus reducing Cu substrate roughness, and decreasing the dendrite-edged graphene grain boundaries by working in a diffusion-limited growth regime. Oxidized Cu foils are utilized due to the lower substrate surface reaction barrier that accelerates the growth rate. Figure 3 clearly shows graphene grains sized over 500um before coalescence. Since the sensing area of the graphene EGFETs is 25 x 75 um^2 – much smaller than the grain size – the devices can be considered as virtually grain boundary free.

In the second part of my talk I will address the issues related with the fabrication and operation of both EGFET and EMA devices. In particular a lab-on-a-chip (LoC) platform for the detection of complex diseases with potential for multiple target detection in an autonomous and portable fashion, will be introduced (figure 4). Several layouts will be presented, including a LoC chip made of 9 graphene transistors, wire-bonded to the printed circuit board. The PCB is inserted into a connector transmitting the signals from/to the integrated control electronics board, connected to the PC via a USB cable. In another layout, with four sets of 22 transistors, the chip is directly inserted into the electronics control board.

Using EMAs for direct detection of DNA hybridization based on cyclic voltammetry and electrochemical impedance spectroscopy, we achieved detection of a 25 nucleotide long target DNA in the range 5 pM to 50 nM, with single nucleotide polymorphism (SNP) sensitivity.

By recording concentration-dependent shifts in the transistor transfer curve, graphene immuno-EGFETs are able to detect the biomarker MMP-9, Matrix Metalloproteinase 9, in concentrations down to 0.01 ng/mL, in a range up to 10 ng/mL. Compared to existing MMP-9 immunoassays, it has a shorter time to diagnostic since it is based on a simpler label-free protocol.

Using EGFETs as genosensors, with probes consisting of the 25-mer oligonucleotide sequence already used with EMAs, plus a C7-amino modification on the 3’-end that binds to the ester group of the PBSE linker, fully complementary target DNA is detected in a linear range between 1 aM and 100 fM, with SNP sensitivity down to 10 aM. The results are normalized for different initial probe surface densities, estimated by fitting the transistor transfer curves to an electrostatic model relating the observed shift in the charge neutrality point to local gating induced by the negatively charged DNA. The results of this work pave the way for a wide range of application of graphene devices in analyte detection for the health and food industries.

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Figures

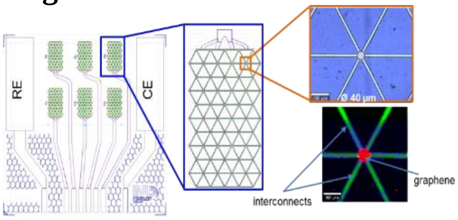

Figure 1: Layout of the EMA and Raman map (bottom right) of one microelectrode.

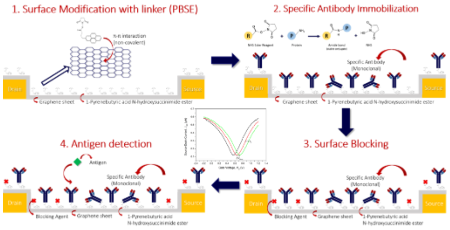

Figure 2: Graphene ISFET channel functionalization steps for biorecognition.

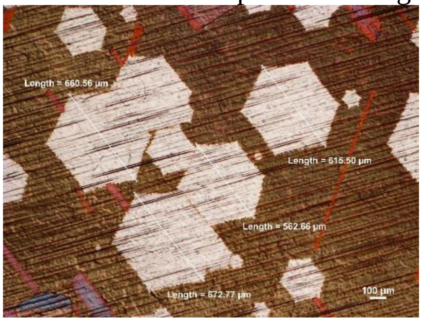

Figure 3: Larger than 500 um grain sized CVD graphene is obtained on Cu catalyst.

Figure 4: LoC made of (from right to left) a 22 graphene transistor chip wire-bonded to the printed circuit board, which is inserted in a connector transmitting the signals from/to the integrated control electronics board, connected to the PC via a USB cable.

The big challenges of small scale fabrication of functional lead free piezoelectric ceramics

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This presentation aims to review the feasibility of small scale fabrication of high aspect ratio functional piezoelectric ceramics through a colloidal approach from aqueous suspensions, as has been already demonstrated in our previous works [1-2]. Lead-containing compounds pose serious environmental concerns and their composition is hard to control in production because of the high volatilization of lead oxide during the sintering process. Alkaline earth-containing compounds are prone to undergo hydrolysis and non-stoichiometric dissolution reactions in aqueous media [3-5]. Preventing such reactions while effectively dispersing the powders to form stable and high concentrated suspensions and is of paramount importance to enhance the performance of advanced functional ceramics [4-6]. Recently we demonstrated how ferroelectric and lead-free piezoelectric ceramics with superior properties could be successfully synthesized and processed in aqueous environments [6-10]. The key issues related to the synthesis, aqueous processing and properties of $BaTiO_3$ (BT), $(Ba,Sr)TiO_3$ (BST), and lead-free piezoelectric ceramics, $0.5Ba(Zr_{0.2}Ti_{0.8})O_3–0.5(Ba_{0.7}Ca_{0.3})TiO_3$ (BZT–BCT) will be reviewed in this presentation.

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Nanoengineering of organic materials for smart and multifunctional applications

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Smart and functional polymers and polymer composites offer large application potential in areas such as sensors and actuators, energy generation and storage, among others. The successful development of applications rely both in the ability to proper tailor polymer properties at a micro and nanoscale and in their implementation by suitable fabrication technologies.

In this sense, printable smart and multifunctional polymers and polymer nanocomposites is an area of increasing interest due to high-performance, simple integration into devices and possibility of obtaining multifunctional materials over large and flexible areas. In this talk, an overview of the main results, strategies and challenges in the development of specific multifunctional materials for areas such as sensors and actuators, biomedicine, environmental remediation and energy storage will be provided.

Plasmonics with graphene

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Invited Speakers

In vitro models for evaluating specific cell responses to graphene oxide and other nanoparticles

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The cooperation between Biomedicine and Materials Science is leading to the development of new nanomedicines based in nanoparticles as carrier systems for specific delivery of therapeutic drugs and diagnostic agents. The evaluation of nanoparticle biocompatibility is an essential prerequisite before their use for these biomedical applications. Taking into account the biocompatibility definition [1], nanoparticles, as any biomaterial, should be nontoxic and generate the most appropriate cellular response. Both *in vitro* and *in vivo* studies must be carried out with cell cultures and animal models respectively, after different forms of nanoparticle administration. In order to evaluate *in vitro* the possible toxicity of graphene oxide (GO) nanosheets and other nanoparticles, we analyze different cell parameters after the treatment of specific cell types with these nanomaterials. These biocompatibility parameters include: cell adhesion and proliferation, cell morphology and cytoskeleton, cell size and complexity, cell cycle phases, lactate dehydrogenase (LDH) release, apoptosis, cell necrosis, mitochondrial activity and intracellular content of reactive oxygen species (ROS) [2]. On the other hand, we also evaluate *in vitro* specific cell responses to these nanoparticles. These specific studies include: endocytic mechanisms of nanoparticle internalization, photothermal effects of GO nanosheets, nanoparticle effects on differentiation and specific activity of osteoblasts and osteoclasts, immune response to nanoparticles evaluating the polarization of macrophages towards M1/proinflammatory and M2/reparative phenotypes and production of cytokines [3-5].

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

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In this study we present a scientific and technological alternative for photovoltaic applications based on innovative ferroelectric oxides like the Bi_2ZnTiO_6 (BZT) perovskite. This material is specifically designed to exhibit a narrow energy band gap (<1.5 eV) and high polarizability. The combination of these properties can be used to easily generate photon-stimulated electron-holes pairs and then to prevent recombination of charge carriers by the intrinsic electric field. Moreover, the use of non-toxic oxides (Bi, Zn, Ti, O) and non-contaminant methods, like thin films deposition by rf-sputtering, assures an environment-friendly technology. Though this promising material was predicted in 2009, a very slim number of experimental works has been published, since bulk BZT phase requires high pressure and high temperature to be synthesized. The presented structural, optical and piezoresponse results demonstrate that it is possible to synthesize polycrystalline tetragonal Bi_2ZnTiO_6 phase onto standard Pt/Si substrates, compatible with standard nano-electronic fabrication and envisaging R&D of photovoltaic sensors and solar cells devices.

Reflections on localized corrosion of metallic alloys and corrosion protection strategies

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Alloys are used in a wide variety of applications in industry. A set of metallurgical processes is involved in alloys production in which a diverse microstructure builds up including different constituents, dispersoids, precipitates etc. Thanks to the tailored microstructure alloys possess valuable mechanical properties. However, when alloys are placed in an aggressive environment consisting of water, salts and corrosive gases, alloys are subjected to degradation and accelerated dissolution of alloy's matrix. This process is called corrosion and normally involves chemical and electrochemical processes. Atmospheric oxygen, having a higher standard reduction potential of oxygen reduction half-reaction, greatly accelerates corrosion of metals causing oxidation of less stable metals. General and localized corrosion are among many forms of corrosion. While the former implies a gradual dissolution of the metal, the latter one reflects selective dissolution of metals at specific local zones and is much more dangerous. Alloying elements constituting intermetallics in alloys may have quite different susceptibility to local corrosion and kinetics of electrochemical processes than the base metal in the alloy.

This work discusses how intermetallics affect localized nature of corrosion in metallic alloys and possible measures for corrosion prevention. Atomic force microscopy (AFM) based methods are powerful tools for detection of intermetallics nature and analysis of their kinetics of corrosion. The susceptibility to local corrosion of intermetallics can be studied by scanning Kelvin probe force microscopy (SKPFM), while kinetics of local corrosion can be studied by in situ AFM. Identifying mechanisms of corrosion of intermetallics allows for development of appropriate strategies for corrosion prevention. These strategies include passive and active protection. The latter approach uses corrosion inhibitors for curbing local corrosion. By mixing both strategies and employing nano-materials tailored for delivery of inhibitors a novel direction such as self-healing materials for corrosion protection is created. Examples of such were demonstrated in protection of aluminum alloys.

SYNTHESIS AND CHARACTERIZATION OF PURE AND DOPED ZnO NANOPARTICLES FOR PIEZOELECTRIC APPLICATIONS

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High performance piezoelectric nanoparticles are the futuristic materials for next generation multifunctional nanosensors, nanogenerators and mamory devices. Versatile ZnO exhibits interesting piezoelectric, pyroelectric, ferromagnetic, semiconducting, optical, etc. properties and have become the focus of intensive research due to their unique nanoscale applications.

In the present talk, our recent results in respect of synthesis and characterization of pure and rare earth (e.g. Cr, Eu, Gd, Y, etc.) doped ZnO nanorods will be presented [1-4]. In ZnO nanostructure, uniform nanorods of diameters down to 20 nm and length around upto 200 nm have been synthesized by low temperature chemical route and their structural, morphological, optical, ferro-/piezoelectric properties were investigated. Effects of various dopings on aforementioned properties of ZnO were investigated. It has been found that the ferroelectric transition temperature changes in the range ~50 ^{o}C to more than 300 ^{o}C while piezoelectric charge coefficient can be enhanced from 10 to more than 400 pm/V (in Y-ZnO) making them useful in high performance nanogenerator applications. The ultra-high piezo-response was linked with change in morphology from nanorods to nanosheets. Further, week ferroelectric and ferromagnetic properties were also observed in doped ZnO nanorods which gave the possibilities of storage and sensor devices at higher temperatures. The synthesized ZnO nanoparticles were used to fabricate energy conversion devices in which electrical energy was generated by simple tapping and folding of fingers.

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Diphenylalanine Peptide Nanotubes with Different Chirality: Structures, Properties, and Applications

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Chirality is one of the fundamental parameters of the hierarchical structure formation of different biomacromolecules. The primary structures of all amino acids exist in two different chirality: L (left) and D (right). Self-organized macromolecules also tend to form hierarchical structures with an alternation of the sign of chirality in the transition to a higher hierarchical level. Depending on the conformation of the primary structure (L or D), the properties of the material also change. One example of such macromolecules is diphenylalanine (FF). Diphenylalanine is one of the self-assembled peptides which have recently become a focus of intense research in nanotechnology [1] because of their unique assembly characteristics and properties such as high rigidity, unique optical properties related to quantum confinement of electrons and holes, appreciable thermal stability as well as exceptional piezoelectric effect [2] and ferroelectricity. As known, in biological nature, almost all amino acids are L. This choice is due to evolution process, but their reason is not enough clear yet. To find some physical sources of such difference, the experimental and theoretical investigations of two types of FF peptide nanotubes (PNTs), based on L-FF and D-FF, were performed.

Both types of PNTs were fabricated by standard method [3]. Data obtained from single crystal X-ray diffraction experiments clearly show the hexagonal structure of the main elementary unit of FF PNT and 12 water molecules in the center [4]. Based on these results a similar molecular model was constructed. Simulation showed that the L-FF has much higher dipole moment and polarization compared to D-FF. These results give some evidence for L-isomers, which have better stability and higher coupling with electric field as compared to D-chiral form. The developed models can be used for further studies of the hexagonal water confinement in PNTs to explain some experimental data. One of the main structural differences of these FF PNTs is that, in the case of alfa-helix, conformation inside PNTs cavity is mostly empty and, therefore, it is preferable to take more water molecules. Experimentally observed FF structures (L and D) also show their origin from FF in alfa-helix, but not from beta-sheet. Models proposed for FF PNTs with water molecules inside the tube based on hexagonal clusters need further study. The main issue is to obtain the best agreement between the modelling results and experimental data.

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Selective Two-Photon Absorption in Carbon Dots: an extra piece of the puzzle of photoluminescence emission

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Carbon dots are an attractive platform for biomedical applications (imaging, sensing, drug-delivery) due to their optical properties, water solubility and ease of functionalization. [1] In this presentation, emphasis will be laid upon our recent study on the nonlinear emission spectroscopy of nitrogen-doped carbon dots. We found that both linear and nonlinear emission can be understood based on the existence of isolated sp^2 clusters involved in $\pi-\pi$ stacking interactions with clusters in adjacent layers, with the biphotonic interaction being selective towards sp^2 clusters bearing electron donor and acceptor groups on the edge. Our comprehensive study provides an extra piece of the puzzle of the origin of photoluminescence emission in carbon dots.

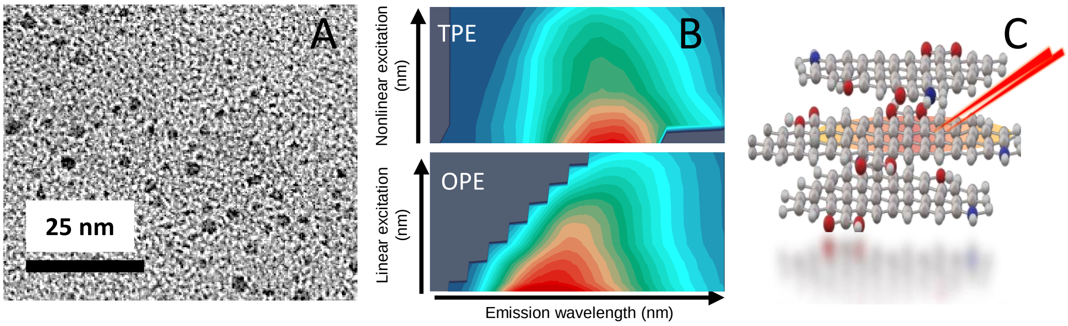

Figure 1. Carbon dots structure and emission spectroscopy: A, TEM image, B, contour plots of the excitation dependent two-photon and one-photon induced emission and C, cartoon of the structure of C-dots.

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Statistical mechanical modeling of the glass structure

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Glasses are disordered materials non-equilibrium materials and their properties evolve continuously as they relax toward their corresponding metastable equilibrium liquid state. Investigations into the structure-property relationships of silicate glasses are of great importance for understanding a broad range of magmatic processes in earth science and for compositional design and process optimization of commercial glasses and glass-ceramics (GCs). However, understanding the structure-property relationships has been for a long time done by empirical modeling, which had a lot of limitations. In recent years, statistical mechanical modeling of glasses has shown promising results.

Therefore, In this work, a new model is derived to determine the distribution of silicate units in glasses (or liquids). The model is based on statistical mechanics and assumes grand canonical ensemble of silicate units which exchange energy and network modifiers from the reservoir. This model complements experimental techniques, which measure short-range order in glasses such as nuclear magnetic resonance (NMR) spectroscopy. By the combined use of the statistical mechanical modeling and broken ergodicity, we shed light on the mechanism of structural relaxation as understood by NMR spectroscopy. Further, the model has potential in calculating the amounts of liquid-liquid phase segregation and crystal nucleation, and it can be easily applied to more complicated compositions.

Mechanical properties and adhesion of the thin films of phase change memory materials

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The purpose of this work was investigation of the mechanical and adhesion properties of GST225 layers deposited by the different methods on the different materials.

Thin GST225 films were deposited by two methods: thermal evaporation in vacuum (TEV) of the synthesized GST225 material, and magnetron sputtering (MS) of the monolithic polycrystalline GST225 target. Thicknesses of the films deposited on different sublayers (Al, TiN , TiN+W, NiCr) were about 130 nm.

According to Energy Dispersive X-Ray Analysis (EDX, CAMEBAX, Cameca) and Auger spectroscopy (Perkin Elmer PHI-660) deposited films have integral composition close to that of GST225. However, according to Auger spectroscopy distribution of the elements along the film thickness is very different.

According to resistivity and differential scanning calorimetry (DSC–50, Shimadzu) measurements crystallization temperature are lower for the TEV films. In addition, DSC scans for this kind of films shows extra peaks, which are absent for MS films. Resistivity is higher in the case of MS films.

Mechanical properties were estimated from the load-unload displacement curves obtained by nanoindentation (nanoindentor B-J53), and analyzed by Oliver and Pharr method.

Atomic force microscopy (AFM Multimode Nanoscope (IV) MMAFM-2) was used for evaluation of the adhesion properties. In most cases adhesion force is higher for the magnetron films, and films with Al, and NiCr sublayers.

So. mechanical properties of GST225 thin films were investigated. It was shown that peculiarities of elemental distribution due to the deposition method can sufficiently influence the properties of GST225 films.

Scanning tunneling microscopy of surface states in topological insulators

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The surface states of topological insulators represent a manifestation of bulk topological order, and in this sense they are distinct from conventional surface states [1]. However, the symmetry of the surface plays significant role in formation of the surface states [2]. The dispersion of topological surface states is a massless Dirac cone. The surface states are non-degenerated in spin due to a strong spin-orbit interaction. The topological surface states are robust against backscattering and, hence, are not sensitive to crystal lattice defects. However, defects in surface crystal structure also lead to a local break of surface translational symmetry and can modify the surface states. Usually, the surface states localized in few nanometer in thick layer at the surface.

Scanning tunneling microscopy is very powerful tool for investigation of a surface with high spatial resolution. A short review of STM study of the Sb(111) topological surface states dispersion is presented. STM investigation of Sb(111) surface crystal structure reveals surface areas obtained both by cleave the surface via break of van der Waals and covalent bonds. The last resulted in creation of a defect layer in a vicinity of the surface with a crystal structure different from Sb bulk crystal structure. DFT simulations reveal formation of structure similar to topological soliton [3].

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Nanoscale studies of ionic conductor materials by strain-based scanning probe microscopy

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Strain-based scanning probe microscopy is a set modes of scanning probe microscopy (SPM) where application of voltage to the SPM tip cause surface displacement registered by SPM tip. For example, electrochemical strain microscopy (ESM) is used for studying the ionic mobility in materials of ionic conductors. The realization of the method is based on Vegard displacement of the surface under the action of charge carrier's concentration gradient stimulating by the biased SPM tip. In this work, we present a novel quantitative approach for the probing of local diffusion coefficients and ion concentration based on frequency dependences of the electromechanical signal in ionic conductors. We provide the theoretical basis considering the dynamic behavior of ion migration and relaxation and change of ion concentration profiles under the action of the electric field of the SPM tip. The analysis of ESM images by the proposed approach allows not only simple visualization but also a quantitative mapping of the ionic diffusion coefficients and the concentration in ionic conductors. The results are validated on Li-battery cathodes ($LiMn_2O_4$) of commercial batteries (Robert Bosch GmbH.) [2].

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Synthesis of Nanofibers by Blow-Spinning Technique and their Potential Applications

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The aim of this work is to present the potential use of the recent Blow-spinning technique (BS) to produce Nanofibers as an alternative to the well-known electrospinning technique [1]. Here, polymeric and ceramic fibers were successfully produced using the BS [2-3]. The fibers were obtained from poly (vinylpyrrolidone) solutions by using isopropyl alcohol as solvent. A systematic study on the influence of solution parameters (concentration, viscosity and solvent) and experimental parameters (injection rate, air pressure, needle size) on the formation and morphology of the fibers was performed to determine the best conditions for synthesis. The results showed no changes in the polymer properties due to the spinning process. The composite fiber polymer/ceramic precursor were thermal treated at different conditions in order to determine the best conditions to produce different kinds of ceramic fibers, such as ferroelectric $LiNbO_3$ and superconductor $Bi_2Sr_2Cu_1Ca_2O_x$ fibers. Studies of x-ray diffraction (XRD) and scanning electron microscopy (SEM) were performed on ceramic samples to determine their structural characteristics, composition and final microstructure. The results shown that desired phases were successfully obtained and the dielectric and superconductor properties was investigated. Additionally, the potential use of different kinds of fibers to fertilizer delivery in agriculture and water treatment will be discussed.

Figure 1: Polymeric fiber (a) and Ceramic fibers (b) produced by Blow-spinning.

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Reduced graphene oxide-based materials for neural regeneration at the injured spinal cord

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Graphene family nanomaterials have emerged as novel biomaterials with properties that overcome those of common materials to date.[1] Electrical and thermal conductivities, customizable features at the nanoscale and mechanical compliance with soft tissues are some of the most relevant features for biomedical applications. One of the fields in which these properties might improve the therapeutic outcome of biomaterials is neural tissue engineering including neural repair strategies for spinal cord injury.[2] Despite multidisciplinary efforts, there are no available therapies to date able to cure this pathology, which dramatically compromises the quality of life and life expectancy of the patients.

In our laboratory, we focus on the exploration of graphene oxide-based materials for the design of novel biomaterials with potential interest in repairing the injured spinal cord. Our studies initially comprised 2D thin films and posteriorly evolved to 3D porous foams composed of reduced graphene oxide (rGO). From *in vitro* tests with embryonic neural progenitor cells[3] to *in vivo* implantation studies in cervical hemisected rats,[4] we are collecting biological evidences from neural tissues that support the idea of these rGO-based materials as attractive biomaterials to support repair in neural tissues.

This project has received funding from MINECO and the *Fondo Europeo de Desarrollo Regional* (MAT2016-78857-R, AEI/FEDER, UE).

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Graphene nanocomposites in chemical catalysis and energy-related electrocatalysis

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Graphene materials, including pristine graphene, oxidized graphene and heteroatom doped graphene, are revolutionizing the way high performance devices are designed and fabricated, particularly in the areas of sustainable energy and environmental technologies.[1,2] From environmental remediation and sensing to energy conversions and storage, there are numerous effective cases of graphene-based materials applications.[3] Graphene materials are typically coupled with other active materials as a nanocomposite. With their outstanding properties the interface with graphene benefits the bare materials by actually emphasizing their properties. To achieve this, the strategy of surface functionalization of graphene with inorganic materials (e.g., metal nanoparticles, oxides, semiconductors), holds the key to enabling the fabrication of high performance nanocomposites. The resultant nanoarchitectures should yield the highest achievable properties and should be unique to the specific applications.

This talk provides a bottom-up approach encompassing the design of graphene-based nanocomposites and their selected applications in high performance systems relevant to chemical catalysis and energy related electrochemical reactions. Heteroatom-doped graphene was studied in the selective reduction of nitro- into amine-arenes, with high catalytic activity and stability/reusability. Furthermore, several graphene nanocomposites with metals oxides: mixed valence cobalt/manganese oxide, phosphomolybdates and phosphotungstates have been successfully applied in energy-related electrochemical reactions involving hydrogen and oxygen evolution reactions (HER and OER, respectively), as well as oxygen reduction (ORR).

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Cavitation as tool to modify and enhance materials surface properties in Nano and Micro level

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Introduction:

Cavitation is the phenomenon of sequential formation, growth and collapse of millions of microscopic vapor bubbles (voids) in the liquid. The collapse or implosion of these cavities creates high localized temperatures roughly of 14000 K and a pressure of about 10000 atm or results into short-lived, localized hot–spot in cold liquid. Thus, cavitation serves as a means of concentrating the diffused fluid energy locally and in very short duration, creating a zone of intense energy dissipation [2]. It may occur at the entry to pumps or at the exit from hydraulic turbines in the vicinity of the moving blades. The dynamic action of the blades causes the static pressure to reduce locally in a region that is already normally below atmospheric pressure and cavitation can commence. The phenomenon is prominent by the presence of dissolved gases that are released with a reduction in pressure.

Cavitation may cause performance problems in fluid power systems. For example, efficiency of a system may be reduced due to cavitation also the level of vibration is increased as a result of the cavitation. At the same time the system noise level is increased as cavitation bubbles collapse. One of the remarkable consequences of cavitation is cavitation erosion [14]. has practical application in the marine industry as a means of reducing drag, enabling objects and hydrofoils designed to function in super-cavitating flows can achieve extremely high speeds. The biomedical industry is investigating its application in the treatment of certain diseases such as cancer. Even some forms of marine life use cavitation to catch their prey.

Cavitation is also used in industry for homogenization such as processing milk, Cavitation is also being researched for use in water purification. Cavitation can even be used to purify water by using its destructive power to breakdown harmful substances into non-toxic compounds. A kind of cavitating jet uses cavitation to destroy harmful compounds.

Cavitation can be generated either by a decrease of the ambient pressure or an increase of the liquid velocity to a point where the local pressure is below the vapour pressure of the liquid at given temperature. As an example the vapour pressure of water at 20 °C is 2.3 kPa. At this temperature and at atmospheric pressure water can bring to 14 m/s before cavitation can occur whereas at 10ºC this limit velocity can reach 20m/s. [7]

The specific geometry of a hydraulic machine will produce local variations of velocity and pressure related to flow curvatures and inertial centrifugal forces. To characterize this range of pressure or velocity that a machine can sustain before cavitation occurs; a dimensionless parameter has been defined called cavitation number σ sigma. The lower sigma, the larger is the cavitation risk.

Related to classification of caviation; there are many ways of classifying the different appearances into types; we may distinguish between four different kinds of cavitation based on creating process such as ; (1) Hydrodynamic cavitation is produced by pressure variations in a flowing liquid due to geometry of the system., (2) Acoustic cavitation is produced by sound of waves in a liquid due to pressure variations.,(3) Optic cavitation is produced by photons of high intensity (laser) light-rupturing a liquid, and (4) Particle cavitation is created by any other elementary particles, e.g. proton rupturing a liquid, in test chamber. The first two kinds produced as a result of tension in the liquid, and the others are achieved by a local deposition of energy [9].

Cavitation can form in various forms based on flow conditions and geometry, such as Traveling Cavitation, Sheet Cavitation (*Fixed cavitation*), Super-Cavitations (*Fixed cavitation*), Cloud Cavitations, Vortex Cavitation, and Ring Cavitation (traveling cavitation)

The cavitation phenomenon features are influenced by many parameters, these parameters are classified into two categories; the *fluid quality"fluid properties"* and *flow quality*. The first category includes working fluid temperature, fluid viscosity and the concentration of dissolved gas in the fluid, while the second category includes the the geometriacl and hydrodynamic conditions of the system.

Becouse of the cavitating jet method has many advantages over the other methods used for the studying the cavitation behaviour, cavitation as tool testing/modification of materials and other application. The apparatus is small. The testing times can readily be adjusted and reduced by choosing a suitable up stream pressure. The results can then be scaled up or down provided the cavitation no. is kept constant, the greatest advantage is the fact that, the flow parameters can be controlled independently.

Abstract: The lecture will present a long investigation work using cavitating jet generator "high speed submerged cavitating water jet generator" which can be summarized as

(1) Different techniques were used for the analysis of cavitation early damage and erosion obtained by using cavitating jets. These techniques varied between the classical and contemporary ones, starting from macroscales to optical methods, subsequently using microscales, and finally arriving to nano techniques. The appropriate comparisons were done and they showed significant results.

(2) Experimental setup with submerged cavitating jet has been used for the study of influences of material, exposure time and working fluid temperature on the damage process. Additionally, comparison of experiments with nitrated and non-nitrated material has been made in order to study the enhancement (mostly reflected as the prolonged incubation time) of erosion resistance achieved by nitrating the specimen surface. The effects of the hydrodynamic parameters (cavitation number, exit-jet velocity and upstream pressure) and in addition of the nozzle geometry and dimensions were also point of investigation. The geometrical and hydro dynamical parameters have strong influences on the, damage, erosion rate, eroded area and depth of erosion. The results for both the non-dimensional standoff distance and the non-dimensional aspect ratio reveal their strong influence on the erosion rate and erosion area. The largest erosion and its pattern depended on the angle of attack, showing a clear maximum at 105°. Comparisons of the results obtained for different cases give highlights and elucidate some of the mechanisms involved in cavitation and erosion and their relations with the tested parameters. The conclusion of the analysis shows that these parameters are very important for the performance of cavitating jets.

(3) In order to demonstrate and establish a possible application of the cavitation phenomenon as an efficient method to modify surface properties. Three FCC (Face Centered Cubic) materials were subjected to high speed submerged cavitating jets under certain working conditions, for time periods between 15 and 1,800 s. The force generated by cavitation is employed to modify the surface roughness in nano and micro scales. The target surface was investigated with digital optical microscopy, atomic force and electrostatic force microscopy (AFM and EFM) and also with a white light interferometer. These different observation techniques indicate that at short exposure times, the observed characteristic features in the microstructure – hills, holes and wavy configuration – can be related to the start of the plastic deformation of the specimen surface. Longer exposure times inevitably result in a greater number of jet specimen interactions leading to specimen erosion and fracture. The results demonstrate the possibility to use cavitation bubbles as a micro- nanofabrication method for the surface preparation/modification or shoot-less surface peening. EFM results present a possibility of using cavitation as tool to enhance the electrostatic properties of a metal surface by modifying its roughness. The degree of enhancement depends on the material properties.

(4) An attempt was made in order to understand the behavior of severely erosive cavitation clouds by collecting visual information about a high speed submerged water jet using several different cameras: Nikon digital camera (Nikon Coolpix 990(E990)), 4-Quik CCD camera and PHOTRON APX (high-speed video camera, 100,000 frames per

second). Visualizations were done for different hydrodynamic conditions, different geometrical parameters and with different techniques in order to be able to understand the jet behavior and its features. The collapsing of bubbles could not be captured because of inadequate temporal resolution of illuminating and recording system, and the huge number of the bubbles in the cloud cavity (chain production).

(5) The attempt to record the sono-luminescence (SL) phenomenon associated to the collapse of bubbles in cavitating jet was also done. The attempts were taken once at different values of cavitation number and once at different working fluid temperature T. Capturing the luminescence phenomenon indicates that collapsing of the bubbles takes place everywhere in the jet path even in the deflected rings. In addition, this proved the existence of spherical bubbles even for this highly turbulent flow.

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Graphene oxide: a basic unit for the controlled self-assembly of 3D carbon macrostructures by supercritical CO_2

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Graphene oxide (GO), is a graphene derivative with peculiar atomic arrangement, which is based on an aromatic carbon 2D macromolecular structure with a high diversity of oxygen functional groups. This singular conformation of GO allows the appearance of several interesting properties, such as aqueous processability, easy surface functionalization, amphiphilicity, high specific surface area and outstanding mechanical and optical properties. Consequently, the interest to explore GO in many different application fields have been growing considerably in the recent years.[1]

New synthetic strategies have been widely explored for the development of advanced functional graphene-based materials that consists on explore GO as a molecular building block material for the controlled assembly into 3D macrostructures.[2] Two main configurations of GO macrostructures have been highlighted in recent years, namely GO free standing paper and porous three-dimensional (3D) macrostructures, showing a high potential for many different applications that range from energy, environment to healthcare.[3]

This work reports for the first time the controlled synthesis of GO aerogels using supercritical carbon dioxide (scCO_2) technology.[4] The synthesis of GO aerogels occurs preferentially by direct self-assembly of dispersed GO sheets in ethanol, using exclusively low temperature scCO_2 technology and avoiding the use of reducing or cross-linking agents. The main advantage of this method is that gelling and drying steps are performed in only one stage of reaction, under mild conditions of pressure and temperature. The scCO_2 process has been optimized regarding the different experimental parameters (temperature, stirring and CO_2 flow) for the controlled final structure of the 3D GO macrostructures. Moreover, this new method allowed to produce mechanically stable non-reduced GO aerogels while using the advantages of efficient, environmentally friendly and low-cost process.

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Exploring the catalytic reaction mechanism of metal oxide additives loaded hydrogen storage system MgH_2

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Abstract:

Nb_2O_5 and TiO_2 additives are known to promote the low temperature hydrogen storage behavior of MgH_2 but the additive-host interaction mechanism remains not understood in the literature. In this context, we herewith explore the details regarding the chemical interaction of Nb_2O_5 / TiO_2 additives with MgH_2 and highlight the most common features existing in these systems. A correlation between in-situ formation of Nb/Ti metal dissolved MgO and ab/de-sorption improvement is noticed in both Nb_2O_5 and TiO_2 loaded MgH_2. The existence of metal dissolved MgO phase is overlooked for years by research community because of its crystallographic resemblance with neat MgO. We believe that this observation is a significant milestone in the area of catalysis.

Introduction:

Among the solid state materials in the 200–400 °C operational category for hydrogen storage, MgH_2 is the only reversible high capacity hydride (7.6 wt.%). Since pure MgH_2 desorbs only a trace amount of H at 300 °C, it requires an additive loading/size tailoring treatment for improved system performance[1]. Metal oxide additives are of particular interest owing to the fact that the reduction of oxides provide considerable variations to sorption surfaces. Note that, it is essential to analyze various metal oxide additives loaded MgH_2 and study what is the most significant common feature connects these systems. Such a correlation study will provide interesting clues to establish a general reaction mechanism for metal oxide additives loaded MgH_2. In this line, we investigated Nb_2O_5/TiO_2 additives for MgH_2 and observed that formation of Nb/Ti dissolved MgO rock salt type phase is the critical step in the catalysis of both systems. These observations lead us to believe that the oxidized magnesium layer existing in the metal oxide additives loaded MgH_2 is not necessarily a barrier layer that passivates the particle surfaces[2]. The existence of metal dissolved MgO phase is overlooked for years by research community because of its crystallographic resemblance with neat MgO. We believe that this observation is a significant milestone in the area of catalysis.

Results and Discussion: We have made composite mixtures of MgH_2+nNb_2O_5 (n= 0.083, 0.10, 0.123, 0.167, 0.25, 0.50, 1.0 and 1.5) and analyzed the mechanochemical reaction products of these in three sets of reaction times, such as, 1h, 10h and 30h (totally 24 samples). After this, a best composition, i.e. MgH_2+0.167Nb_2O_5 was studied by varying the reaction time viz, 2 min, 5 min, 15 min, 30 min, 45 min, 1h, 2h, 5h, 10h, 15h, 20h, 25h and 30h. The X – ray diffraction (XRD) and high resolution transmission electron microscopy (HRTEM) studies suggest that a well dispersed "unidentified product", ´x´, resembling the crystallographic features of MgO rock salt, with an average size of 3-5 nm starts forming after 1h reaction time. This product ´x´ was then used as an additive for MgH_2 (3 wt.%) and the effect was studied by differential scanning calorimetry (DSC) and Sieverts volumetric techniques. These studies proved the excellent catalytic activity of ´x´ over MgO and Nb_2O_5 for MgH_2. Following these observations the next system MgH_2+xTiO_2(x = 0.25, 0.33, 0.5 and 1) has been investigated under similar experimental conditions. Reduction of titania, resulting to evolution of a monoxide rock salt nanocrystalline phase was identified by in-situ X-ray diffraction (XRD) performed for a 3 mol.% titania loaded MgH_2 sample. Existence of homogeneously distributed Ti in a crystalline rock salt matrix ($Mg_xTi_yO_{x+y}$) was confirmed by combined analysis of XRD, HRTEM and elemental chemical mapping techniques. Moreover, titanium in Ti^{2+} valance state was confirmed by XPS study. DSC study and hydrogen storage measurements proved that the Ti dissolved MgO promotes the low temperature dehydrogenation of MgH_2. These observations reiterate that the MgO rock salt layer existing in oxide additives loaded MgH_2 is not necessarily a barrier layer that blocks the diffusion of hydrogen.

Conclusion:

It is clear that the chemical reduction of additives Nb_2O_5/TiO_2 and subsequent formation of in-situ active species is the most important step in the catalysis of TiO_2/Nb_2O_5 additives loaded MgH_2

system. Since Nb_2O_5 and titania are the model oxide additives for MgH_2 known in the literature, it is likely that the best metal oxides behave the same way as Nb_2O_5/TiO_2. It is also necessary to investigate the catalytically less active/ inactive metal oxides to analyze if in-situ formation of $Mg_xM_yO_{x+y}$ rock salt formation is indeed the case only in the best performing systems.

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Oral presentations

Porphyrin@GO hybrid materials as DNA G-quadruplex detectors and stabilizers

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G-quadruplex (G-Q) folding at the telomeres of deoxyribonucleic acid (DNA) promotes the inhibition of telomerase, an enzyme present in almost 90% of human tumor cell populations.[1,2] Although the tetracationic 5,10,15,20-tetrakis(1-methyl-pyridinium-4-yl)porphyrin (TMPyP) has suitable dimensions to match, induce and stabilize G-Q,[3-5] a major drawback is related with its lack of selectivity over common duplex DNA.[6]

In this work were developed non-covalent hybrids between TMPyP and graphene oxide (TMPyP@GO) and their potential for the selective detection and stabilization of G-Q were evaluated. The formation of such hybrids was monitored through UV-Vis and spectrofluorimetric titrations and Raman mapping was applied for the first time to provide new insights on the molecular interactions present in this type of hybrids. The interaction of these hybrids in the presence of DNA oligonucleotides able to fold into duplex (abb.: 4GC) or G-Q (abb.: $(T_2AG_3)_4$) was studied through spectrofluorimetric titrations. The most prominent change was the selective fluorescence recovery observed during the titration of TMPyP@GO with G-Q resembling a "turn-off-on" fluorescent, as illustrated in ***Figure 1.*** This result suggests that upon addition of oligonucleotide sequences that are able to form G-Q structures, the porphyrin molecules are progressively detached from the GO sheets of the non-covalent hybrids, giving rise to a fluorescence recovery. This distinctive behaviour was not observed when free porphyrin was titrated with both types of DNA oligonucleotides, allowing us to conclude that the introduction of GO nanoplatforms may represent a new way to introduce selectivity for G-Q stabilization. Therefore, we believe that these hybrid nanoplatforms can pave the way for a new class of antitumor drugs based on the delivery of porphyrins for G-Q stabilization.

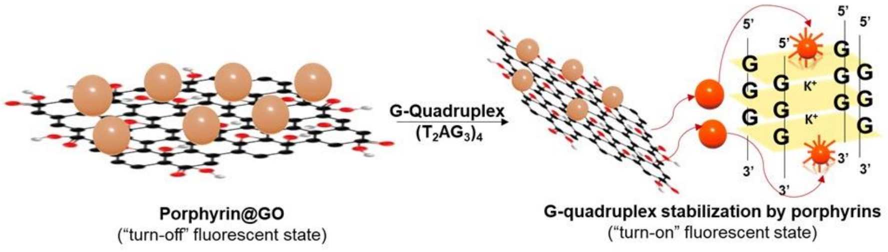

Figure 1 – "Turn-off-on" fluorescent model. The TMPyP@GO hybrid as a quenched fluorescence ("turn-off" state), but upon addition of DNA G-Q structures, the porphyrin molecules are progressively detached from the GO sheets of the non-covalent hybrid in order to stabilize G-Q, giving rise to a fluorescence recovery ("turn-on" state).

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On the vibration behavior of rotating nanostructures

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- In this work, authors have addressed one of the most important topics of nanomechanics that combines between mechanical engineering, materials science and nanotechnology; the recent advances in this filed led to many novelties and findings in the field of nano/micro electromechanical systems (NEMS/MEMS) [1]. The dynamic behavior of rotating nanostructures based CNTs working as nanomotors, nanoturbines, nanoshafts [2], nanobearings, nanorobots and other nanoscale devices and machines applied in medicine, biology, defense, aeronautical and electronic industries. In order to understand and master the mechanical properties of nanomaterials under different dynamic conditions, this study investigates the free vibration of rotating nanostructures based single walled carbon nanotube considered as a simply supported Euler-Bernoulli nanobeam.

- The present work aims to investigate the free vibration of Euler-Bernoulli nanobeam based single-walled carbon nanotube (SWCNT), by using the theory of nonlocal elasticity that has been introduced by Eringen [3] in 1972. The governed equations of motion are developed after derivation using Hamilton's principle; the discretization of the Eigen system is done using a semi analytical procedure called Generalized Differential Quadrature Method (GDQM) [4, 5], which is very efficient for nanoscale engineering problems. Unlike other famous numerical methods such as finite element method and difference method that need high performant computational resources and much time, GDQM is very easy to get involved and programmed by engineers and researchers.

- Authors solved the following Eigen problem:

$$(-\lambda^2[M] + j\lambda[G] + K).(U, V, W)^T = 0$$

The novelty of this work is the study of the spinning of nanostructures; authors also showed that SWCNTs undergoing rotation have exceptional behavior, where the small scale has a significant effect on the frequency parameters and angular velocity.

- From the obtained results, authors summarized the following conclusions:

  - The rotation inertia of the SWCNT nanostructure have split the frequency parameter to forward and backward frequencies (Campbell diagram).
  - The increase critical speed parameter influences the forward frequency parameter increasingly and the backward frequency parameter decreasingly.
  - The small scale parameter has a significant effect on the dynamic parameters; it decreases the frequency parameters as it increases.

- Authors have limited their study only for simply-supported nanobeam because the recent studies [6, 7] indicated that the differential form of Eringen's nonlocal theory leads to accurate results only for fully simply-supported boundary condition.
- Findings of this study can be involved in the design of next generation nanomachines and nanodevices.

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Statistical Analysis of Variation of Cavitation Cloud Characteristics in Space and Time and Related Behavior Based on the Flow Condition

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Cavitation clouds show an unsteady periodic tendency with frequencies depending on the flow conditions. In a cavitating water jet flow with cavitation clouds, the cavities or the clouds produce high impact at their collapse. In order to make the mechanism of the periodic cavity behavior clear, we experimentally examined the behavior of the cavitating jet (cavity clouds) and the jet generator. The cavitation clouds were visualized in a high-submerged cavitating water jet by a high-speed camera photography. Injection pressure, nozzle diameter and geometry, nozzle mounting (for convergent and for divergent flow) were varied as influencing parameters. The consecutive images extracted from obtained movies was processed using a custom Matlab program. The variation of geometry and dimensions of the cavitating jets with time were analyzed statistically. The effect of upstream pressure and nozzle geometry is investigated from a viewpoint of steady and unsteady behavior of a cavitating water jet (cavity clouds). As a result, it was found that the cavitating flow has oscillation pattern in the cavity geometry and dimensions (thickness, length, area etc) with time. The corresponding periodical oscillation of the cavitation clouds has been analyzed. Frequency of the oscillation was determined by the analysis of the clouds' shape. Additionally, dependence of this frequency on injection pressure and nozzle geometry has been analyzed. This isolation is related to the upstream pressure fluctuation caused by the plunger pump and the interaction between the jet and the surrounding which lead to characteristic oscillation of cavitation clouds accompanied with the shedding, growing, shrinking, regrow and discharging and collapsing process of the clouds.

Poster presentations

P1

Ferroelectric physical properties of various dipeptide nanotubes

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Recent investigation and molecular modelling of the formation, structure and physical properties of various types of the peptide nanotubes (PNT), containing different amino acids, are presented and discussed in this work. The nanotube formation by various hydrophobic dipeptides and its structural properties were studied by many authors [1, 2]. But, their physical properties were studied not enough. The main focus was concentrated on diphenylalanine (FF) nanotube, which demonstrated unique physical properties, such as, piezoelectricity and ferroelectricity, and these properties were studied most detailed [3]. Nevertheless, the others PNT can exhibits some specific similar properties. For example, the branched-chain amino acids (BCA) can support ferroelectricity in such structures as liquid crystals [4, 5] and transmembrane ion channels [6]. From other side, not only FF, but such BCA as leucine (L) and isoleucine (I) in their dipeptide structure (LL, II) revealed the nanotube formation [1]. These simple compounds crystallize with hydrogen-bonded head-to-tail chains in the shape of helices or rings with four to six peptide molecules. The resulting structures have chiral hydrophilic channels with a van der Waals diameter up to 10 A. These peptide-based nanotubes had attracted considerable interest as model for membrane channels and pores [6]. Followings studies found the ferroelectricity in FF PNT [3, 7]. But other PNTs were not enough studied in this matter.

In present work the ferroelectric properties of various PNT are investigated using molecular modelling by quantum semi-empirical PM3 methods (HyperChem package). The various conformation (α and β) and chirality (L and D) were modelled and the PNT ferroelectric properties were studied. Data obtained show the formation of the strong polarization along main OZ axis for all PNTs. The most strong polarization was found for II PNT (Pz = ~ 6 $\mu C/cm^2$), while for LL PNT Pz = ~3.6 $\mu C/cm^2$. As it was known for FF PNT the biggest polarization (for chirality L and conformation β) is Pz = ~4 $\mu C/cm^2$ [3, 7]. Therefore, data obtained shown that II PNT could have the most promising interest for further application as more strong ferroelectric compound. The others PNT ferroelectric properties (dielectric permittivity, piezoelectric coefficients, etc.) are analysed too in compare with some known and available experimental data.

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P2

MoS_2 flakes stabilized with DNA/RNA nucleotides: *In vitro* cell response

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Two-dimensional (2D) nanomaterials, in particular, transition metal dichalcogenides (TMDCs), such as MoS_2 and WS_2, have recently emerged in science as nanomaterials with potential use in biomedicine because they have unique structures and distinctive properties [1,2]. One of the most fascinating ways to favor the interaction of nanomaterials with biological systems is the use of proper biomolecules as exfoliating/dispersing agents. In his study, we investigate the biocompatibility of MoS_2 flakes from stable colloidal aqueous suspensions stabilized through adsorption of nucleotides [adenosine monophosphate (AMP), guanosine monophosphate (GMP) and flavin mononucleotide (FMN)] [3]. Particularly, the cellular response of undifferentiated cells (MC3T3-E1 preosteoblasts) and human sarcoma osteoblasts (Saos-2) exposed to such dispersions in a range of concentrations has been explored. The response of the nucleotide-stabilized MoS_2 flakes on the viability and cell proliferation, on the production of intracellular reactive oxygen species (ROS), and on the preosteoblast differentiation process has been evaluated, as well as the incorporation of the nanomaterials by MC3T3-E1 and Saos-2 cells. The nucleotide-stabilized MoS_2 flakes were found to exhibit excellent biocompatibility, allowing their cell proliferation and maintaining high cell viability. Moreover, their incorporation was observed in both types of cell, without affecting the integrity of the cell plasma membrane, which makes them ideal candidates for delivering drug/gene directly into cells. Results revealed that the ROS production by both cell types could be related to the biomolecule used as dispersing/stabilizing agent (AMP, GMP and FMN mononucleotides) in the colloidal dispersion of MoS_2 flakes. The *in vitro* cell response of tumoral cells to these nanomaterials differs from that of undifferentiated cells, which provides the basis for their potential use in cancer photothermal therapy at the sub-cellular level.

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P3

Hydroxyapatite with defects by first-principles calculations

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Hydroxyapatite (HAp) is an important component of mammal bones and teeth, being widely used in prosthetic implants. Despite the importance, several other promising applications involving this material (photo-catalysis, electronic and optical properties), is not clear enough. But on all these properties are very influencing by various HAp defects. The ideal HAP structure is well know - HAp have two main crystallographic space group structures: hexagonal $P6_{3/m}$ and monoclinic $P2_{1/b}$. HAp in the body of the living organisms are as a biological, rather than a mineral material. This means that their structure differs from the perfect crystal structure of pure HAp. Their difference from an ideal pristine HAp mineral consists in their stoichiometry and defects, such as oxygen O and OH group's vacancies, interstitials of hydrogen H, various atomic impurities and substitutions of several atoms, which change the electronic band structure and all that relates to it, including the band gap width, optical properties [1, 2]. Recent computational study of HAP structures, containing several types of defects. clearly show these influences [3]. But it is not enough, because needs more correct and precise calculations.

In this study a new exchange-correlation treatment to the calculations of several properties of the pristine and defective HAp with several defect types of the O vacancies from PO4 group and OH, as well the full OH group vacancy, were considered. The properties of HAp are considered using semi-local PBE potential and B3LYP hybrid exchange-correlation functional. The excitation properties are compared with the results of GW-approximation method for calculation of quasi-particle band structure. It was shown that optical properties of bulk HAp are best described using B3LYP exchange-correlation functional, while the optimization of structures are better doing PBE [4, 5]. The data obtained by this new computational methodology show that all these defects create the additional electron energy levels Ei (Kohn-Sham energy levels) inside band gap Eg, which influence on the optical and photocatalytic HAP properties, because it changes the effective band gap for the electron photo-excitation. More exact calculation of this optical processes can be made by calculations of the electro-electron correlation of the excited electron states with the Frank-Condon relaxation taken into account.

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P4 (SC1)

Synthesis and antimicrobial and cytotoxic activities of silver nanoparticles synthesized from Streptomyces palmae OF1 strain

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Purpose: The aim of the present study was to use actinobacteria as a biological system for synthesis of silver nanoparticles (AgNPs) with special reference to their antibacterial and antifungal activities as well as toxicity toward mammalian cells. Due to the development of multi-drug resistance in microorganisms against available antibiotics and limited cancer therapies, there is an urgent need for alternative therapies to combat resistant pathogens and cancer [1]. Actinobacterial strain was chosen for synthesis of biogenic nanoparticles because these microorganisms are known to be important producers of most natural bioactive compounds [2].

Materials and methods: BioAgNPs were characterised by UV-vis, Fourier transform infrared spectroscopy, Zeta potential and, Nano tracking analysis, and Transmission electron microscopy. Antimicrobial activity of AgNPs synthesized from *Streptomyces palmae* OF1 strain against bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Klebsiella pneumoniae* and *Bacillus subtilis*) and fungi (*Candida albicans* and *Malassezia furfur)* was evaluated alone and in combination with antibiotics by using micro-dilution method. The minimum inhibitory concentration (MIC) and minimum biocidal concentration (MBC) of AgNPs and antibiotics were determined. Synergistic effect of combined antibiotics and AgNPs was evaluated by Fractional inhibitory concentration index determination (FIC). The MTT assay was performed for cytotoxic activity of AgNPs alone and in combination with antibiotics towards mouse fibroblasts (3T3) and HeLa cell line.

Results: Analysis of physico-chemical properties revealed that silver nanoparticles were spherical, small in size (5-20 nm) and polydispersed. The lowest MIC of AgNPs was found against *P. aeruginosa* (16 µg ml^{-1}), followed by *C. albicans* and *M. furfur* (32 µg ml^{-1}). The synergistic effect of combined antimicrobial agents against bacteria and fungi was found (FIC=0.12). The IC$_{50}$ values of AgNPs towards 3T3 and HeLa cell lines were found to be 4.0 µg ml^{-1} and 3.8 µg ml^{-1}, respectively.

Conclusions: The synthesis of AgNPs using *Streptomyces palmae* OF1 strain is an eco-friendly, cheap and nontoxic method. The antimicrobial activity of AgNPs could result from their small size. Remarkable synergistic effect of antibiotics and AgNPs offer their valuable potential in nanomedicine for clinical application as a combined therapy in the future.

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P5

Local piezoelectrical properties of P(VDF-TrFE)/ Graphene and P(VDF-TrFE)/ Graphene oxide composite fibers

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Piezoelectricity in macromolecule polymers has been gaining immense attention, particularly for applications in biocompatible, implantable, and flexible electronic devices. This paper describes composite fibers of copolymer poly trifluoroethylene wiz. (P(VDF-TrFE)) with graphene (G) and graphene oxide (GO). Experimental and theoretical investigations were done to understand the effect of the G and GO concentration on polarization behaviors of bulk composites and composite fiber microstructures. The electromechanical properties of the PVDF/G and PVDF/GO nanofibers are investigated in terms of piezoresponse mapping, local hysteresis loops, polarization reversal by advanced piezoresponse force microscopy (PFM) and Kelvin Probe Force Microscopy (KFM). For understanding the mechanism of piezoresponse evolution of the composite we used models of PVDF chains, interacting with Graphene/GO layers, its behavior in electrical field and computed the data for piezoelectric coefficients using HyperChem. Experimental results qualitatively correlate with obtained in the calculations.

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P6 (SC2)

Efficiency of cationic surfactants with polyamine platform as corrosion inhibitors of stainless steel and carbon steel

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The aim of the present research is to determine the correlation between the structure of new gemini surfactants, their physicochemical properties and their protective properties [1]. Investigated compounds contain a esters groups which strongly affect on biodegradation. The effectiveness of the inhibition properties of these compounds was determined performing 24-hour and one week tests by potentiometric measurements and using electrochemical impedance spectroscopy. The morphology of the stainless steel and carbon steel surface before and after immersion in the electrolyte (3M HCl / 3.5% NaCl) was examined using confocal laser scanning microscopy and scanning electron microscopy.

The main parameter to determine in the use of amphiphile structures (which posess surfactants) as corrosion inhibitors is the CMC value. Concentration is a main factor to affecting to corrosion inhibitor efficiency. Below the CMC, individual molecules begin to adsorb on the metal surface. Around the CMC concentration, micelles are formed on the solution and also a monolayer forms on the protective material [2]. Any addition of surfactant to the solution will not increase too much the corrosion inhibitor efficiency as the entire surface of the material is already saturated.

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P7

Double MgO/FeCoB interface free-layer for perpendicular magnetic tunnel junctions: effect of thickness and spacer

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The perpendicular magnetic anisotropy (PMA) provided by the interface between the FeCoB free layer and MgO tunnel barrier is the basis of the perpendicular magnetic tunnel junction (pMTJ). To increase the free-layer volume, and thus the data retention, while keeping the PMA, two FeCoB/MgO interfaces are used [1].

Improved switching speed is expected by setting the free layer's magnetization in an easy-cone state [2]. Such an easy cone requires a negative second-order PMA term, $K2 < 0$, and is observed in the crossover from out-of-plane to in-plane anisotropy [3,4]. Here we explore the easy-cone state in double-MgO free layers using the ferromagnetic resonance technique (FMR).

MgO/FeCoB/X(0.2 nm)/FeCoB/MgO free layers were prepared with X = Ta or W spacers. We show that the insertion of a metal spacer allows an easy-cone state to be preserved at increased thicknesses of double-MgO free layers, for which the thermal stability is enhanced. Particularly, the W spacer enables higher K_2 values than Ta. While K_1 is still to be improved to meet MRAM's thermal stability requirements, these layers may already be useful for spin-torque oscillators.

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P8

Improved functional properties of co-doped $BiFeO_3$ compounds

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INTRODUCTION

Complex manganese and iron oxides characterized by a metastable structural and magnetic state are of particular interest caused by their rich phase diagrams and promising physicochemical properties perspective for developing of new efficient functional materials. The metastable state of the crystalline and / or magnetic structure is accompanied by an increased sensitivity of such compounds to external influences, such as electric and magnetic fields, mechanical stresses, temperatures, etc. Formation of compositions with a metastable structure has been achieved by the authors using the chemical substitution schemes for the initial oxides $LaMnO_3$ and $BiFeO_3$ by rare earth and alkaline earth ions. In order to understand how La and Mn substitution affects the crystal structure and magnetic behavior of the compounds near the phase boundary, extensive diffraction and magnetometric study of the $Bi_{0.86}La_{0.14}Fe_{1-x}Mn_xO_3$ ($x \leq 0.15$) perovskites have been carried out.

EXPERIMENTAL/THEORETICAL STUDY

$Bi_{0.86}La_{0.14}Fe_{1-x}Mn_xO_3$ ceramics with the compositions near the rhombohedral-orthorhombic phase boundary were prepared by solid state reaction using high purity oxides. X-ray and neutron diffraction measurements have approved phase purity of the compounds, attested an occupation and position of the ions and have confirmed the designed chemical formulas. X-ray diffraction patterns were collected using a Bruker D8 diffractometer, neutron powder diffraction (NPD) measurements were carried out at Helmholtz-Zentrum Berlin. The magnetic properties of the samples were investigated using PPMS set-up.

RESULTS AND DISCUSSION

X-ray diffraction measurements performed for the $Bi_{0.86}La_{0.14}Fe_{1-x}Mn_xO_3$ (x=0.05, 0.1, 0.15) have confirmed the absence of any impurity phases in the materials under study. The samples with x=0 are known to possess single-phase rhombohedral structure with the R3c symmetry permitting spontaneous polarization. The XRD pattern collected for the compound with x=0.05 has been successfully refined using a two-phase structural model suggesting the coexistence of the major (~90%) polar rhombohedral and minor (~10%) antipolar orthorhombic phases. An increase in the Mn concentration leads to a rapid increase in the fraction of the antipolar phase at the expense of the rhombohedral phase. Indeed, in the $Bi_{0.86}La_{0.14}Fe_{0.9}Mn_{0.1}O_3$ compound, the antiferroelectric phase has been found to be dominant (~80%). A further increase in the Mn content results in a vanishing of the R3c phase. The narrow concentration range determining the two-phase region at room temperature points at the high chemical homogeneity of the solid solutions and supports the choice of the synthesis conditions used to prepare the samples. An increase in the temperature up to 900 K stabilizes the nonpolar orthorhombic $GdFeO_3$-type structure (space group Pnma) which is considered as a typical high-temperature phase characteristic of bismuth ferrite based materials. The initial structural state of the x=0.05 and x=0.1 samples recovers upon cooling back to room temperature. The x=0.15 compound maintains its monophasic anti-polar orthorhombic state up to 840 K.

Magnetization measurements of the $Bi_{0.86}La_{0.14}Fe_{1-x}Mn_xO_3$ samples confirm that Mn substitution dramatically affects the magnetic structure of lightly-doped $Bi_{1-x}La_xFeO_3$. The substitution with Mn ions affects the stability of the cycloidal order in the ferroelectric phase of the $Bi_{1-x}La_xFeO_3$ multiferroics and induces transformation from the antiferromagnetic to weak ferromagnetic state. A decrease in the spontaneous (or magnetic-field stabilized) room-temperature magnetization taking place in the $Bi_{0.86}La_{0.14}Fe_{1-x}Mn_xO_3$ system with an increase in the Mn concentration correlates with the NPD data which suggest the lowering of the Neel temperature with increasing of dopant content.

CONCLUSION

The substitution of manganese ions in $Bi_{0.86}La_{0.14}Fe_{1-x}Mn_xO_3$ tends to suppress the existing polar displacements and stabilizes the antiferroelectric $PbZrO_3$-like structure. The polar and antipolar phases coexist at $0.05 \leq x \leq 0.1$. Depending on the initial phase composition at room temperature, the ferroelectric phase can be either fully or partly recovered by heating. The heating-induced transformation is not irreversible. Magnetic measurements supplemented the results of the diffraction study indicate that the combined substitution affects the stability of the cycloidal antiferromagnetic order in the polar phase and can be considered as a promising approach towards designing magnetoelectric multiferroics with the polar phase- related spontaneous magnetization.

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P9

Preparation, stability and local physical properties of P(VDF-TrFE)/Graphene oxide composite thin films and nanofibers

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Piezoelectric polymer nanocomposites have gained extensive attention in the past decade due to the improvement of the physical properties, such as higher moduli, improved thermal properties, and better barrier properties compared with the original polymer matrix. Here we describe composite materials (thin films and fibers) of copolymer poly trifluoroethylene wiz. (P(VDF-TrFE)) with graphene oxide (GO). The obtained microstructures were investigated locally using piezoresponse force microscopy (PFM) and Kelvin Probe Force Microscopy (KFM). The switching behavior, charge states, piezoelectric response, self-polarization and dielectric permittivity of the composites were found to depend on the concentration of GO. Moreover, taking the Advantage of the nanometer scale resolution of Atomic force microscope (AFM) and KFM, the method is able to give insight on charge propagation by monitoring the surface charge potential distribution on two-dimensional microstructure surface.

For molecular modeling and quantum-chemical calculations by HyperChem 8.01 package we used models of PVDF chain, its behavior in electrical field. Our theory modeling show possibility uses our models for understanding the mechanism of piezoresponse evolution of the composites.

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P10

Improving surface properties and porosity of electrospun scaffolds for cartilage tissue engineering

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Polycaprolactone (PCL) electrospun scaffolds have long been used for cartilage tissue engineering applications due to their biocompatibility, biodegradability, good mechanical properties and easy processability. However, their inherent hydrophobicity prevents cell adhesion and cell proliferation. On the other hand, natural polymers, such as gelatin, have been reported to support cell adhesion due to its hydrophilic character and the presence of cell recognition sites. Another common limitation of PCL electrospun scaffolds is their inherent small pores, which can hinder cell migration. The introduction of a sacrificial agent on the scaffolds, such as polyethylene glycol (PEG), which can be co-electrospun with the polymer of interest, has been reported to overcome this limitation. The sacrificial polymer is then dissolved away in water, resulting in an electrospun scaffolds with increased porosity. The present work combines these approaches to improve the surface properties and the scaffolds' porosity that will benefit cell adhesion, migration and proliferation. Thus, a new series of electrospun scaffolds composed of PCL, gelatin and PEG sacrificial particles were fabricated and characterized on their chemical composition, wettability, topography and biocompatibility using an articular cartilage progenitor cell line. According to the results obtained, the addition of gelatin led to an increased hydrophilicity of the scaffolds, which resulted in better cell adhesion and proliferation. The introduction of PEG sacrificial particles enlarged the pore size of the scaffolds to values comparable to the cell diameter and allowed cell migration through the scaffold.

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P11

Cell seeding process optimization on polycaprolactone-gelatin-arcade-like-architecture-scaffolds

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The articular cartilage (AC) is a highly specialized tissue that exhibits anisotropic mechanical properties due to its structural organization that varies with depth. Because it is an avascular tissue, the regeneration capacity of cartilage tissue is limited. This situation, may lead to degeneration of cartilage in cases of injury, which limits not only the normal functioning of the articular cartilage but also the surrounding tissues. In this context, cartilage tissue engineering has been focusing on the development of methods aimed at achieving better results, like the growth of tissue in three-dimensional porous structures and implantation of the same in the affected site. The aim of this work is to optimize the seeding process of cartilage cells on specific scaffolds. For that, to better mimic the cartilage native structure, fibrous scaffolds of polycaprolactone (PCL) and Gelatin with distinct fiber orientation were produced by electrospinning. The incorporation of cells in the 3D architectures was performed using: a top and bottom pipetting procedure; an injection method with a syringe; and a compression technique. The validation of the results was performed through the measure of cell metabolic activity via a resazurin assay**.** By the analysis of the results, cell proliferation was detected, suggesting that these scaffolds are biocompatible and could provide a favorable microenvironment to the adhesion and growth of the tissue. Regarding the seeding techniques, the compression approach presented the highest cell viability, followed by top and bottom approach, indicating that the incorporation of cells was assured and potentiated through these techniques.

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P12

A biomimetic tissue-engineered scaffold for repairing the injured spinal cord: a proof of concept

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Repairing the injured spinal cord is probably one of the most difficult challenges of modern medicine since available palliative, pharmacological and rehabilitation treatments have proved to be inefficient to completely restore the lost autonomous, motor and/or sensory functions of patients worldwide [1]. Thus, in recent years, tissue engineering (TE) scaffolds are emerging as central players for complex regenerating strategies due to their ability not only to deliver powerful drugs capable of inhibiting the appearance of scar tissue, but also to enhance the cell response towards a substantial anatomical and physiological recovery of the injured area [2]. In this work, we propose a biomimetic 3D TE scaffold able to provide two complementary porous and fibrous topographies with the purpose of recreating *in vitro* the morphology of the grey and white matters, respectively. Preliminary results confirmed that the scaffold presents an architecture that match its natural counterpart and, additionally, that the inclusion of graphene as a key biomaterial optimizes the chemical and mechanical properties of the scaffold, boosting the cell-material interactions [3].

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P13

Polycaprolactone-gelatin-graphene oxide electrospun nanofibers for tissue engineering applications

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In recent years, tissue engineering (TE) has emerged as a promising approach to complete the deficient natural regeneration processes of the central and peripheral nervous systems and consequently attenuate some devastating physical, psychological and social consequences for patients worldwide. The success of neural TE strategies deeply rely on the combination of biomaterials with advanced nanofabrication techniques towards the fabrication of fibrous scaffolds able to present a biomimetic topography and a high surface area/volume ratio capable of enhancing the cell response and/or the delivery of drugs [1]. The excellent physicochemical properties of carbon-related nanomaterials, such as graphene, have encouraged their exploitation for neural regeneration. Complementary to the ground-breaking electrical, optical and mechanical properties of graphene, graphene oxide (GO) presents a highly oxygen functionalized surface, which impart a hydrophilic character to the material and consequently leads to excellent biologically features [2]. Thus, in this work, we fabricated a wide range of composite electrospun polycaprolactone-gelatin-GO scaffolds to study the influence of concentration, size and reduction level of GO on the chemical, mechanical and morphological properties of the fibers with the final purpose of identifying the best compositions to be included in future neural cell culture protocols involving electrical stimulation.

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P14

8-hydroxyquinolinium hydrogen squarate crystal: a new piezoelectric and NLO active crystal

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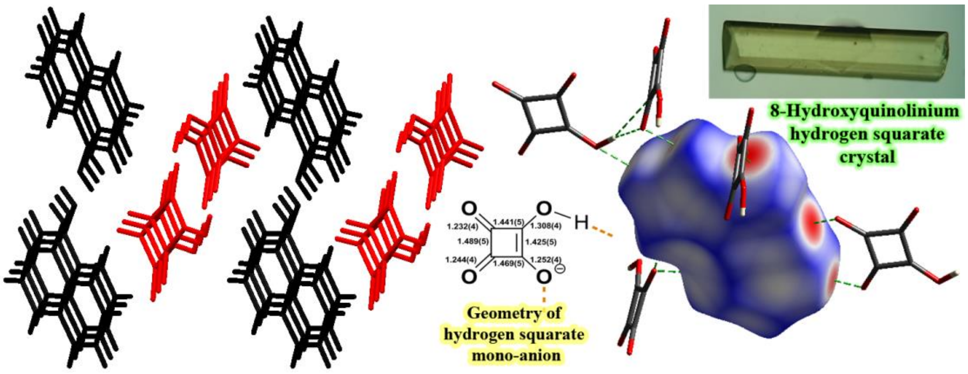
A novel 8-hydroxyquinolinium hydrogen squarate (HQS) crystal (1:1 molecular complex of 8-hydroxyquinoline with squaric acid) has been synthesized by slow evaporation technique and characterized by single crystal X-ray diffraction, UV-vis, photoluminescence, dielectric, piezoelectric, SHG studies and by DFT calculations. Structurally, the HQS crystal contains one hydrogen squarate mono-anion ($C_4HO_4^-$) and one protonated 8-hydroxyquinoline cation ($C_9H_8NO^+$).The crystal packing of HQS crystal illustrates that the high tendency of N-H···O &O-H···O hydrogen bonds and C-H···π interactions leads to 3-D expansion of infinite supramolecular chains running parallel to '*b*' crystallographic axis. Hirshfeld surface and fingerprint plot study revealed all the non-covalent interactions present in the HQS crystal system. Indeed, O···H/H···O interactions possess the largest contribution to the overall molecular surface of both the moieties. The significant contributions from O···H/H···O and C···H/H···C interactions indicate the presence of C-H···O, O-H···O & N-H···O hydrogen bonds and C-H···π interactions, respectively. From UV-vis spectroscopy, the lower cut off wavelength was found to be 357 nm and optical band gap was calculated to be 3.11 eV. The PL emission spectrum illustrates violet and blue color richness (417 nm and 474 nm) for the HQS crystal. The SHG conversion efficiency of the HQS crystal was found to be 2.6 times of standard KDP sample. The HQS was found to exhibit a low value of dielectric constant (~6.9) at room temperature at higher frequencies. The optimized molecular structure, UV-vis spectrum and HOMO-LUMO energy gap were found to be in a good agreement with experimental values. The piezoelectric coefficient was measured as 3 pC/N. The experimental results demonstrated that the HQS crystal is a novel promising crystal for NLO and piezoelectric applications.



P15

Crystal growth and characterizations of flux grown MPB compositions of ferroelectric PZN-PT and PMN-PT single crystals

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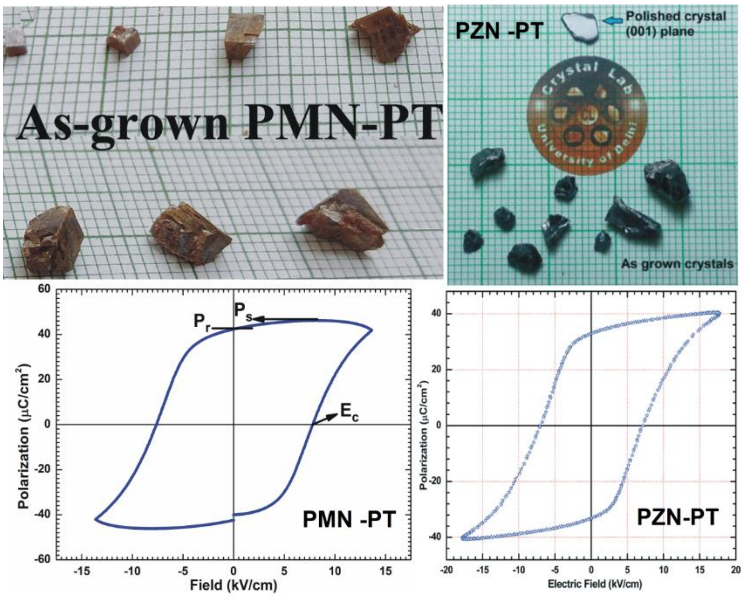

Ferroelectric single crystals of $Pb(Zn_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$ (PZN-PT) and $Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PMN-PT) have been successfully grown in the vicinity of morphotropic phase boundary, using flux technique where $PbO+B_2O_3$ were used as flux. Dielectric, ferroelectric, piezoelectric and pyroelectric properties of both the crystals were studied. A high Curie temperature (T_c = 190 °C) was observed for PMN-PT crystals compared to PZN-PT (T_c = 131 °C) in the dielectric study. The converse piezoelectric coefficient (d_{33}^*) of PMN-PT was obtained using the slope of displacement vs. voltage curve (butterfly loop) and was found to be 1398 pm/V. The direct piezoelectric coefficient (d_{33}) for the PZN-PT crystals was found to be ~ 1000 pc/N, respectively. Good saturated loops were obtained for both the crystals indicating good ferroelectric quality of the crystals. Further, true-remanent hysteresis study was used to unveil the usable polarization value of PMN-PT crystals after eliminating the non-remanent components of polarization. The true (usable) component of polarization switches with the applied field and hence serves as memory component in devices whereas the non-remanent component randomizes as soon as the field is removed. Also, time-dependent compensated hysteresis analysis was carried out to study the resistive-leakage nature of the PMN-PT crystals. A comparative analysis on various properties of PZNPT and PMNPT was presented.

P16

Local piezoelectricity in amino acids microcrystals

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Piezoelectricity is the ability of noncentrosymmetric crystals to produce mechanical stress/strain under electric field or charge under mechanical stress. This property has long been used in acoustic transducers, sensors/actuators, piezomotors, nanorobots, energy harvesters, piezoMEMS and more [1]. Now a research activity on nanoscale materials shifts from inorganic substances to polymers and biology objects. Recently, novel organic and bio-organic materials have been found to be ferroelectric at room temperature [2].

Crystalline amino acids are in form of zwitter ion belonging to the family of hydrogen-bonded crystals and, in some cases, its oxide and phosphate salts have a ferroelectric behavior. From crystallographic point of view the amino acids structures are very interesting from the perspective of ferroelectricity: amino acids are of low symmetry without an inversion center, and many of them belong to the polar groups. This means that these protein amino acids are pyroelectrics and possibly ferroelectrics. However, up to now, only several amino acids which show piezoelectricity are known: glycine and DL-alanine comparable to quartz. L-alanine, L - valine, L- glutamic and DL-tyrosine have much weaker piezoelectric activity [3].

Unfortunately, data on local electromechanical properties of amino acids is limited to experimental data obtained before the development of nanotechnological methods as the atomic force microscopy and its variations as force spectroscopy or piezoresponse force microscopy (PFM) to measure the mechanical and ferroelectric properties at the nanoscale.

In this work we used PFM methods to find out that γ-glycine is not only piezoelectric but also ferroelectric [4]. The pronounced ferroelectricity was confirmed by the visualization of as-grown and artificially created domains, pronounced hysteresis (measured locally and in pressed samples) and by the distinct Curie-Weiss behaviour.

We have found that piezoelectric and ferroelectric domains can be observed on the surface microcrystals of several pure amino acids at room temperature by PFM methods. These domains can be artificially induced by the locally applied electric field via the conducting tip.

Due to the ubiquity of piezoelectricity in biological systems, we show that these microscopy methods allow successfully use at high-resolution electromechanical development of important studies of microcrystal of the amino acids growth on Pt/Si substrates.

Full description of the electromechanics of the "elementary" units of the protein building blocks could bring the further understanding of the molecular biophysical properties of other important biomolecules.

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P17

Multifunctional aerogels based in nanocellulose and graphene-based materials

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During the last decades, cellulose materials, either in the form of films, foams or aerogels have been a topic of great development. For example, cellulose aerogels show great versatility to be used as pollutants absorbers, insulation materials or biomedical devices [1, 2]. However, these aerogels have poor mechanical properties when compared to other materials and present high flammability. To overcome these limitations, in this work we report the preparation of a multifunctional hybrid material by impregnating aluminum (Al) open-cell foams with defibrillated bacterial cellulose (BC) aqueous solution containing graphene-based materials (GBMs). Thus, creating a polymeric foam inside the Al open-cell foam structure. The Al open-cell foam acts as a mechanical support for the cellulose aerogel and the incorporation of GBMs into the cellulose provide not only some mechanical reinforcement but also fire-retardant characteristics [3, 4]. All the prepared foams were fully characterized and special focus was addressed to mechanical, acoustic, thermal and fire-retardancy properties. Results demonstrate that these new hybrid foams are multifunctional materials since they present enhanced thermal insulation and sound absorption properties as well as fire-retardancy. Thus, a novel environmental friendly hybrid solution is presented with potential use for high-end insulation applications.

Aknowdgements

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P18

Discovery of the conductivity behaviour of $CaCu_3Ti_4O_{12}$ by using Scanning Probe Microscopy technique

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High-k dielectrics with colossal dielectric constant (CDC) ($\varepsilon' > 103$) are a matter of great interest since they provide an improvement in the efficiency of electronic devices through the miniaturization of capacitive electronic components. Calcium copper titanate ($CaCu_3Ti_4O_{12}$), a non-ferroelectric material, whose exceptional dielectric properties have been reported in 2000 [1], attracts the attention of scientific community because of its CDC ($\varepsilon' >105$), observed for ceramics and single crystals.

Despite the efforts of the scientific community, a conclusive explanation about the polarization mechanisms that justify the exhibition of CDC is still missing. Discarding the existence of any ferroelectric transition, the experimental data, collected during the last decade, point to an extrinsic barrier mechanism(s) as the origin of the main dielectric polarization. Recently, in a theoretical work, Bueno et al. [2], have indicated a polaronic stacking fault defect model as the origin of the high dielectric constant in $CaCu_3Ti_4O_{12}$ (CCTO) materials. In our work, we present the experimental confirmation for the inhomogeneous conductivity in CCTO ceramics, at the nanometric scale, which can support the polaronic stacking fault defect model as the origin of CDC. Using the Scanning Probe Microscopy technique implemented in the contact Spreading Resistance mode, we have confirmed an insulating behavior of the grain boundaries and, for the first time, revealed a dual behavior of the grain microstructure with a clear coexistence of conductive and insulating nanoscale-patterned in-plane features.

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P19

Porphyrin-based organic-inorganic hybrid on the removal of metal ions

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The presence of toxic heavy metal ions in the environment represents a serious threat to human health, living resources and ecological systems. [1] Therefore, the detection and elimination of heavy metals from natural waters and wastewater is attracting increasing attention. Due to their unique features and properties porphyrins have been explored for detection and removal of metal ions in solution. [2,3] However, the immobilization of ligands on solid matrices is an essential requirement to a more practical and environmentally feasible application, and silica is a promising platform.[4] In this work a novel inorganic-organic hybrid material based on silica chemically modified with a β-formyl porphyrin, with a high metal removal efficiency, was developed. The new material surface exhibits good chemical and thermal stability, and a fast and spontaneous adsorption of metal ions. This adsorbent can be continuously regenerated without affecting its extraction capability and effective ability to remove metal ions from real water samples. [5]

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P20

GRAFENE OXIDE MACROSTRUTURES FOR THE REMOVAL OF HEAVY METALS IN CONTAMINATED WATERS

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The main threats to human health from heavy metals are associated with exposure to lead, cadmium, mercury and arsenic ions designed by potential toxic elements (PTEs). These metals have been extensively studied and their effects on human health regularly reviewed by international bodies such as the WHO (World Health Organization).

Precipitation, oxidation-reduction, membrane filtration, ion exchange, and photo degradation are some of the conventional methods available to remove contaminants from water [1]. Because of its simplicity, versatility and efficiency, adsorption is a very attractive, and the most popular water treatment process [2]. A classical adsorbent is activated carbon, the most relevant from an industrial point of view [3]. Nevertheless, its production cost is elevated and presents a high cost of regeneration.

The development of more efficient and economical technologies becomes imperative. The growing development of nanotechnology and advances in the development of three-dimensional (3D) structures of graphene-based materials has shown that these materials have a high potential in remediation.

Our team [4] studied the possibility of the chemically functionalization of the surface of 3D graphene oxide (GO) structures, in order to increase its sorption capacity or enhance its affinity for a specific pollutant. In particular, we modified the surface of 3DGO with nitrogen functional groups from ammonia (3DGON) increasing its removal efficiency for Hg(II) up to 95% in ultra-pure water with 24 hours contact time. These results were obtained with only (10 mg L^{-1}) of this material, to achieve a residual concentration of Hg(II) in solution very close to 1 µg L^{-1}, which is the European guideline value for drinking water.

Following the improvement of that graphene-based macrostructures we are developing new graphene-based materials with enhanced performance for Hg removal. Different 3DGO surface functionalization is being explored. The common feature of the functional groups under study is the presence of nitrogen. A new composition was already developed showing great affinity for Hg removal from different waters (ultra-pure water, tap water, river water and seawater), at realistic conditions (initial concentration of Hg in water of 50 µg L^{-1}). It was found that 10 mg L^{-1} of material can remove up to 98% of Hg from ultra-pure water in just 2 hours of contact time.

Our aim consists in the optimization of GO-based macrostructures, chemically manipulated to increase their removal efficiency and selectivity towards the PTEs, test the efficiency of these materials in real water (river and sea water) and develop a prototype able to be customized for a specific contaminated water.

Acknowledgment

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P21

Design and fabrication of anisotropic scaffolds towards cartilage tissue engineering

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Articular cartilage degenerative diseases are a huge problem in contemporary society. Cartilage tissue engineering is making possible the creation of biomimetic scaffolds that can mimic the depth dependent nanostructural organization of the fibrous collagen network of the native articular cartilage, with the combination of biomaterials and cells, to find a therapeutic solution for this type of injuries [1]. This study meant to optimize the pore size of the fibrous electrospun zones that comprise 3D anisotropic scaffolds under development in our research group, and also to recombine these electrospun zones in alternative fibrous 3D architectures. By electrospinning of polycaprolactone (PCL) and the combination with a hydrogel of graphene oxide-collagen (GO-collagen), four different fibrous/porous architectures of PCL-GO-collagen scaffolds were created. After a process of lyophilisation, these scaffolds were able to provide a suitable porous network for cell culture protocols. To evaluate the influence of fibres size and orientation on the final properties of the 3D structures, the PCL-GO-collagen scaffolds were characterized morphologically. A preliminary biocompatibility test was made, while the different fibrous zones that compose the scaffolds were assessed with chondrocytes. Biocompatibility testing showed promising results, but on the other hand, also showed that the optimization of the scaffold fibrous zones porosity needed to be continued, so that it can promote/facilitate cell migration through the whole scaffold.

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P22

Porous carrageenan-based carbons for water treatment

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Emerging pollutants in wastewater include vestigial pharmaceutical compounds, such as the antibiotic ciprofloxacin (CPX), that are threats to ecological and human health, and therefore sustainable technologies for their removal are sorely needed. [1, 2] Carbon-based porous nanomaterials are receiving increasing attention due to their excellent performance in several fields, including in the purification of water via adsorption technologies. Furthermore, these carbon nanomaterials allow exploring of other functionalities that are difficult to achieve in commonly available activated charcoal. [3] In this work, we describe carbon nanomaterials that have been prepared via hydrothermal carbonization of carrageenan biopolymers. A detailed characterization of these nanomaterials has shown amorphous carbon spheroids of micro to nanometer size (Figure 1), with a negative surface charge but of low porosity. Further treatment with potassium hydroxide solution resulted in more porous structures, which were then assessed for ciprofloxacin (CPX) removal from aqueous solutions. CPX was used here as an example of a water pollutant due to their extensive use as an antibiotic. In the operational conditions under analysis, 98% of CPX could be removed from water, thus anticipating great potential for activated carbon nanomaterials prepared from renewably source biopolymers for adsorption-based treatment of wastewater.

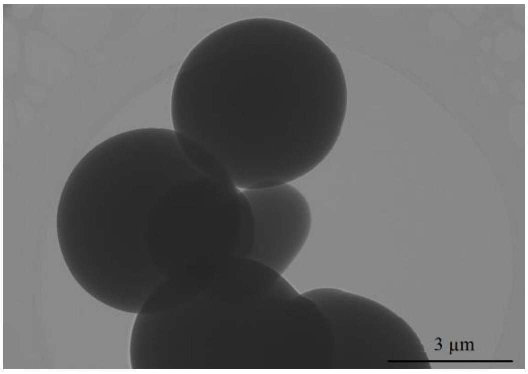

Figure 2 – Transmission Electron Microscopy (TEM) image of carbon spheres, prepared from hydrothermal carbonization of κ-carrageenan

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P23

Development of the contact system for the effective multisectional thermoelements with the operating temperature range from 300 to 1200 K

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One of the ways of increasing efficiency of thermoelectric generators (TEG) is development of the multisectional thermoelectric elements (MTE), which work in the wide temperature range. Important problem of MTE fabrication is providing reliable commutation between sections of the legs of thermoelectric elements (TE), which ensure minimal thermal and electrical losses, and prevent mutual diffusion of elements. In addition, contact system (CS) formed by contacting layers must provide Ohmic contacts with thermoelectric materials (TEM) and between the layers, and must play the role of diffusion barrier with high adhesion strength. So, the aim of the work was development of the structure and fabrication methods of effective CS.

CS was developed for n- and p-type TEM on the basis of Bi_2Te_3 obtained by the electron beam evaporation and magnetron sputtering of Ni and Mo. Resistivity of CS does not exceed 10^{-9} Ohm·m^2, contact adhesion strength is 12-16 MPa.

CS structures to the middle temperature n- and p-type TEM on the basis of Bi_2Te_3, PbTe and GeTe were proposed. CS structures were fabricated by magnetron sputtering of the following layers: W-Ta-N/Ni, Ni/W-Ta-N/Ni, Ni/TiN/Ni. Resistivity of CS does not exceed 10^{-9} Ohm·m^2, contact adhesion strength is 10-16 MPa.

CS structures to the high temperature n- and p-type TEM on the basis of $Si_{0.8}Ge_{0.2}$ were developed. Ohmic contacts and diffusion barrier layers were fabricated by the electron beam evaporation and magnetron sputtering of Mo/Ni and Ni/Mo/Ni. Chemical and electro-chemical deposition metods of Ni were used for the fabrication of commutation layers. Resistivity of contacting systems does not exceed 10^{-9} Ohm·m^2, contact adhesion strength is 16-24 MPa.

Developed CS are used in the construction of MTE with the operating temperature range from 300 to 1200 K.

P24

Morphological characterization of surfaces manufactured by High-speed machining: Fractal approach of surface topography of tibial insert in UHMWPE

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The complex surface geometry in tibial insert of the knee prosthesis, developed by High-speed machining, demands strict surface topography quality requirements, mainly to prevent osteolysis [1]. The fractal analysis is an effective tool in monitoring the milling of these components, since it is a technique sensitive to the self-affinity characteristics of these surfaces [2].

The objective of this work was to propose a method based on the fractal approach for the inspection of surface topography of the tibial insert manufactured by High-speed machining.

Test pieces of tibial insert were prepared by varying the machining strategy. The material used was a UHMWPE. The evolution of fractal values were correlated to cutting tool trajectories and compared to average roughness, *Ra*.

Extended depth-of-field method allowed the ordering of stacks of images obtained from optical microscopy, to quantitative investigation of behavior of surfaces. A method to establish the threshold between different scales for multi-fractal behavior of the machining surfaces was proposed, allowing comparing mono-fractal behavior with mixed fractal.

The fractal analysis machined surfaces of the tibial insert can be successfully conducted from elevation maps resulting by combining conventional optical microscopy and 3-D reconstruction by extended depth-of-field.

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P25

Graphene based sensors for air quality monitoring

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This work focuses on recent advances in the field of graphene-based gas sensors, emphasizing the use of modified graphene that broadly expands the range of nanomaterials sensors [1]. Graphene films were grown on copper by CVD and transferred to arbitrary substrates by using a solution of $FeCl_3$ as copper etchant (Figure 1). After the synthesis, the samples were functionalized with Al_2O_3 by ALD and characterized by a large set of experimental techniques such as XPS, Raman and SEM.
The results clearly demonstrate that graphene was successfully synthesized and transferred to SiO2, glass and a polymer [2]. Moreover, Al2O3 forms homogeneous thin films on graphene allowing its use as a gas sensor [3]. From this perspective, a laboratory prototype device based in measuring the electrical properties of the samples as a function of the gas absorption is under development (Figure 1.1-3). As future work, additional research on the functionalization of graphene will be performed to improve the sensitivity and selectivity of the sensors for air pollutants such as for example VOCs, PM and CO.

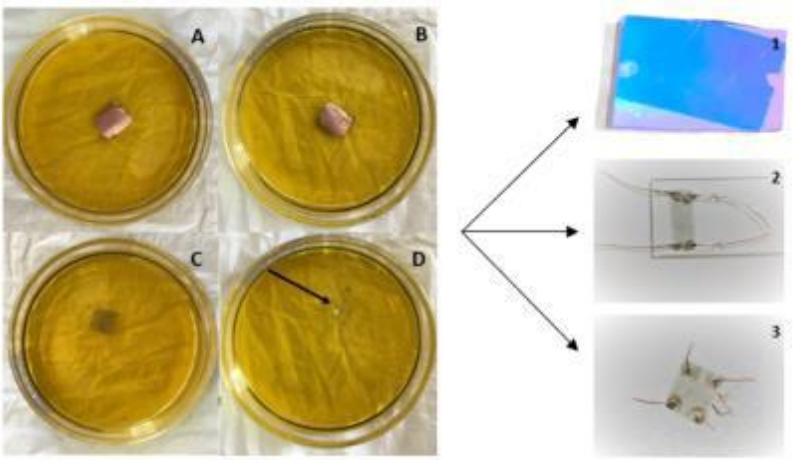

Figure 1 - Transfer of graphene to: 1) SiO2/Si, 2) glass, 3) polymer

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P26

Graphene/MoS_2 vertical heterostructures

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Vertical heterostructures of 2D materials are a promising strategy for developing thin film devices [1]. Among others, vertical stacking of graphene and transition metal dichalcogenides are interesting materials for designing photovoltaics, (bio) sensors, transistors and optoelectronic devices [2]. This poster shows the characterization of graphene on MoS_2 films by photoelectron spectroscopy and atomic force microscopy.

MoS_2 samples were grown following a new set up based on the controlled sublimation of Mo under vacuum conditions and subsequent sulphurization in a CVD system. Afterwards, graphene grown on copper foils by standard CVD protocols were transferred onto MoS_2 films. Complementary, MoS_2 surfaces were also coated with thermally reduced graphene oxide for comparison.

The results indicated that the quality of the MoS_2 samples is comparable to thus obtained by standard CVD process [3]. While graphene transfer process caused a small quantity of defects in its structure, the reduced GO coatings presented a higher level of defects and less homogenous coverage that could affect the efficiency of future devices.

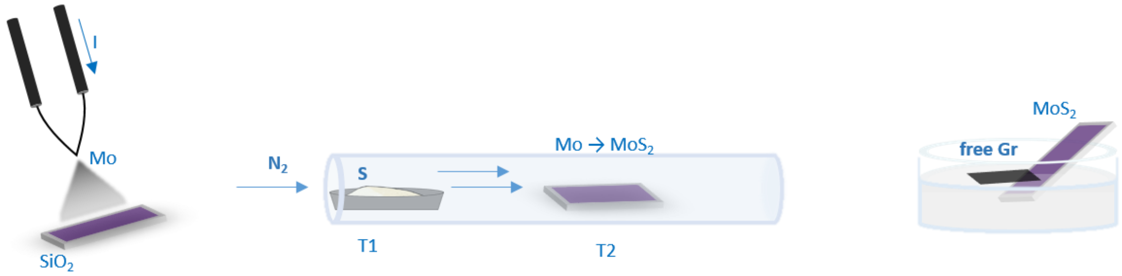

Figure 1: Schematic representation of the preparation of Gr/MoS2 vertical structures.

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P27

Exploring Temperature Dependent Raman and Magnetization in $ErFeO_3$ Single Crystal

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Rare-earth orthoferrites received renewed attention in recent years because of their attractive properties, promising for applications in ultrafast spin switching and spin reorientation transition. In addition, due to the coexistence of ferroelectric and magnetic ordering, they exhibit interesting hybrid properties. These Properties were driven by asymmetric exchange interaction between R-4f and Fe-3d electrons. In this family, $ErFeO_3$ shows a sequence of magnetic transitions in orthorhombic *Pbnm* perovskite structure, during cooling.

In this work, high quality $ErFeO_3$ single crystal was grown by the optical floating zone. The grown single crystal was oriented in the (100) plane. To track magnetic transitions we measured temperature dependent (a) Raman spectra between (80 – 700 K) and (b) magnetization up to 10 T. In Raman analysis different modes corresponding to the perovskite structure were observed and different stages of phase transition are clearly noticed. In magnetic measurements clear change of slope occurred in zero field cooled and field cooled measurements at 4 K and 87 K and these changes correspond to contribution Er^{3+} ions and spin glass transition. The effect of anisotropy on magnetization and exchange bias are analyzed.

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Gamma Irradiation Induced Effect on Ferroelectric Triglycine Sulphate (TGS) Single Crystals

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Transparent and unidirectional single crystals of ferroelectric Triglycine Sulphate (TGS) were grown using Sankaranayanan-Ramasamy (SR) method. The grown crystals have been subjected to Gamma Irradiation using Cobalt-60 as source in different dosages viz, 10-50 KGy. An attempt has been made to study the effects of free Radical formation due to irradiation and their changes in the physico-chemical properties. TGS crystal has been subjected to optical absorption studies and the observed shift in the λ cut-off with respect to dosage was noted. Vibrational analyses like FTIR, Raman studies were performed to assess the vibrational structure of the compound after different irradiation doses. To ensure the presence of free radical the crystal is subjected to Electron Paramagnetic Resonance (EPR) studies. The ferroelectric phase transition and the effect of irradiation on the same, due to the free Radical in the crystals, were assessed from the dielectric studies. The piezoresponse and bulk polarization measurements confirm the drop in ferroelectric polarization and formation of defect centres in TGS after 50 KGy irradiation. The results will be discussed in detail.

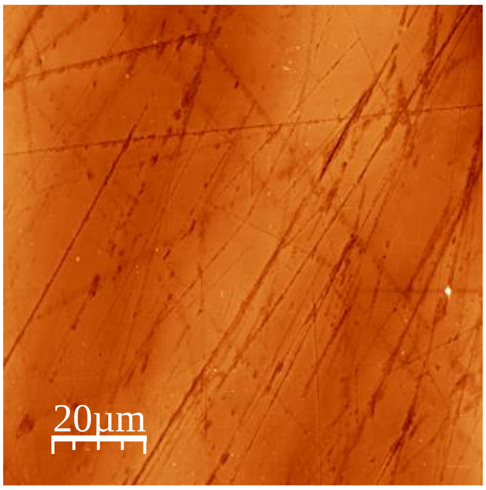

Fig 1. Topography of TGS irradiated at 50 KGy

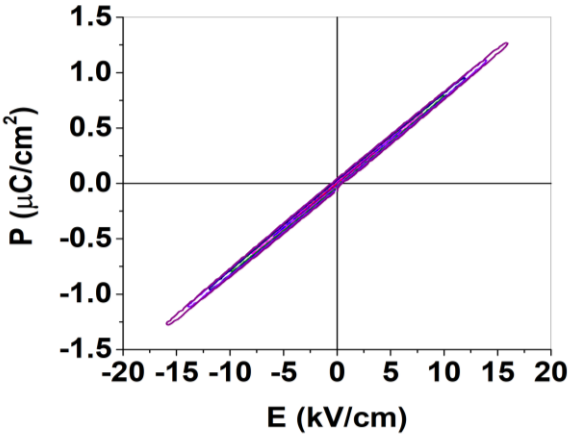

Fig 2. P-E Loop of TGS irradiated at 50 KGy

Notes

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