2nd International Conference on Nanomaterials Science and Mechanical Engineering

University of Aveiro, Portugal
July 9-12, 2019

Book of Abstracts

tema
university of aveiro
centre for mechanical technology and automation

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

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Title
2nd International Conference on Nanomaterials Science and Mechanical Engineering
Book of Abstracts

Editors
Igor Bdikin
Budhendra Singh
Raul Simões

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2nd International Conference on Nanomaterials Science and Mechanical Engineering,
1st Workshop on Characterization and Analysis of Nanomaterials
and
Workshop on Local-scale and magneto-electric measurements in functional nanomaterials
(2nd ICNMSME-2019 / 1st WCANM-2019 / TransFerr-2019)
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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Prof. Dr. Vítor António Ferreira da Costa (UA, Portugal)

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Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques (UA, Portugal)

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Conference Web

http://icnmsme2019.web.ua.pt/

1st Workshop on Characterization and Analysis of Nanomaterials
University of Aveiro, Portugal, July 9, 2019

Auditorium: Anf. 22.3.2 (DEM)

Lectures		
9:00-9:15	**WELCOME ADDRESS: Prof. Dr. António Manuel de Bastos Pereira, Dr. Igor Bdikin**	
9:15-10:15	CHAIR: Dr. Igor Bdikin **Dr. Duncan Paul Fagg,** X-ray diffraction (XRD)	
10:15–10:30	**Coffee break**	
10:30–11:30	CHAIR: Dr. Igor Bdikin **Prof. Dr. José Coutinho,** Modeling of nano-structures	
11:30–12:00	**Bystrov V.S.,** Coutinho J., L.F. Avakyan A.V. Bystrova, E.V. Paramonova (**O2**) Piezoelectric, ferroelectric, optoelectronic phenomena in hydroxyapatite by first-principles and influencing of them by the defects levels	
12:00–12:30	**Dr. Nuno André Fraga de Almeida,** Scanning electron microscope (SEM)	
12:30–14:00	**Lunch**	
14:00–15:00	CHAIR: Dr. Gil Alberto Batista Gonçalves **Dr. Igor Bdikin,** Atomic force microscopy (AFM) and Nanoindentation	
15:00–16:00	**Dr. Gonzalo Guillermo Otero Irurueta,** X-ray photoelectron spectroscopy (XPS)	
16:00–16:15	**Coffee break**	
Equipment / method presentations		
16:15–18:15	**X-ray diffraction**	**NRD Lab**
	High resolution electron microscopy	**NRD Lab**
	Atomic force microscopy and Nanoindentation	**NRD Lab**
	X-ray photoelectron spectroscopy	**NRD Lab**
	Modeling of nano-structures	**Auditorium UA**

Local-scale and magneto-electric measurements in functional nanomaterials

University of Aveiro, Portugal July 9, 2019

Coordinator: Dr. Andrei Kholkin
Department of Physics &
CICECO – Aveiro Institute of Materials
University of Aveiro
Portugal

After decades of intense research, functional nanomaterials are now an integral part of many applications and attract the attention of a large research community. Intrinsically **Aveiro** multi-disciplinary, research activities are spanning from engineering, physics, metrology and chemistry to biology and medicine. Likewise, current applications may differ from contrast agents for medical imaging to touch screens for mobile phones.

The scope of this Workshop is to cover the principles and applications of local scale measurement techniques such as Atomic Force Microscopy (and techniques based on it, e.g. Piezoresponse Force Microscopy, Kelvin Force Probe Microscopy etc.) and HR-(S)TEM for nanomaterials research and provides a forum for presenting and discussing new results.

The workshop is organized in frame of Marie Skłodowska-Curie Research and Innovation Staff Exchange program, projects TRANSFERR and FUNCOAT projects (Grant agreement: 778070 and 823942).

More information about the projects is available at: https://hzg.de/ms/funcoat/ and http://transferr.eu/

TransFerr-FunCoat joint workshop
University of Aveiro, Portugal
Measurement techniques for studying functional nanomaterials
July 9, 2019

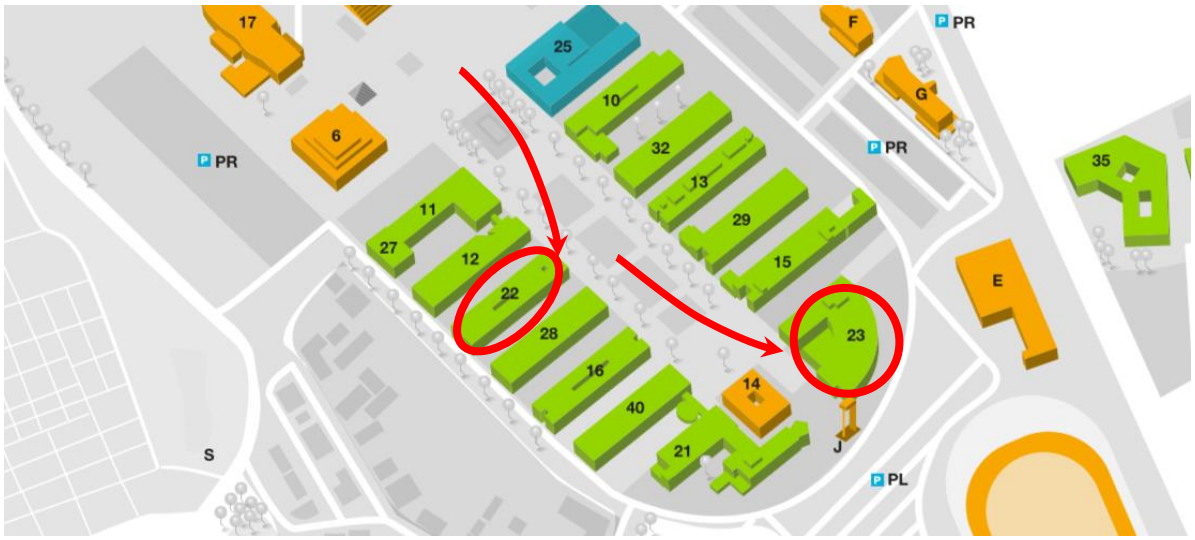
Workshop program
Auditorium: José Grácio (DEM)

9:00 -9:15	CHAIR: Dr. Dmitry Karpinsky Opening Session – Welcome and general info about MSCA-RISE action and FUNCOAT project overview *Dr. Maria Serdechnova (Helmholtz Zentrum Geesthacht, Germany)*
9:15 -9:30	TransFerr project overview *Dr.Andrei Kholkin (CICECO & University of Aveiro, Portugal)*
9:30 -10:00	***Keynote talk*** Near-field microwave microscopy in applications to ferroelectrics and in-situ imaging in liquid electrolytes *Dr. Alexander Tselev (CICECO & University of Aveiro, Portugal)*
10:00-10:20	Coffee break
10:20-11:00	CHAIR: Dr. Andrei Kholkin ***Keynote talk*** Development and design of novel multifunctional PEO coatings *Dr. Carsten Blawert (Helmholtz Zentrum Geesthacht, Germany)*
11:00-11:30	Lecture "Measurements of local electronic and ionic transport by scanning probe microscopy" *Dr. Denis Alikin (University of Aveiro, Portugal)*
11:30-12:00	Lecture "Use of functionalized coatings for environmental protection" *Prof. Rastko Vasilic (University of Belgrad, Serbia)*
12:00-12:30	Lecture "Structural research by photons and neutrons with focus on nano-resolution of P03 beamline" *Dr. Vasyl Haramus (Helmholtz Zentrum Geesthacht, Germany)*
12:30-14:00	Lunch
14:00-14:30	CHAIR: Dr. Svitlana Kopyl Lecture: "Local characterization: Kelvin probe, localized corrosion characterization, role of inhibitors" *Dr. Kiryl Yasakau (University of Aveiro, Portugal)*
14:30-15:00	Lecture:"Magnetic and crystal structure phase transitions in multiferroics" *Dr. Dmitry Karpinsky (SPMRC, Minsk, Belarus)*
15:00-18:00	Practical session/training AFM, PFM, etc.
19:00-21:00	Working dinner

2nd International Conference on Nanomaterials Science and Mechanical Engineering

(SCIENTIFIC PROGRAM)

University Aveiro, DEM, Complexo Pedagógico (auditorium 23.1.7) 09.07-12.07. 2019



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10 July 2019

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<tr><td>9:00-
9:30</td><td colspan="3">WELCOME ADDRESS: Prof. Dr. Vítor António Ferreira da Costa (UA, Portugal), Prof. Dr. António Manuel de Bastos Pereira (UA, Portugal), Dr. Paula Alexandrina de Aguiar Pereira Marques (UA, Portugal), Dr. Duncan Paul Fagg (UA, Portugal), Dr. Igor Bdikin (UA, Portugal), Dr. Gonzalo Guillermo Otero Irurueta (UA, Portugal), Dr. Gil Alberto Batista Gonçalves (UA, Portugal)</td></tr>
<tr><td></td><td colspan="3">Session: New Materials and Advanced Materials
CHAIRS: Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques,
Prof. Dr. António Manuel de Bastos Pereira</td></tr>
<tr><td>9:30-
10:15</td><td colspan="3">Plenary Lecture
Prof. Dr. Philip LeDuc
Planes, Trains, Automobiles….and Cells?
Departments of Mechanical Engineering, Biomedical Engineering, Computational Biology, and Biological Sciences Carnegie Mellon University, USA</td></tr>
<tr><td>10:15-
11:00</td><td colspan="3">Plenary Lecture
Prof. Dr. Yuri Dekhtyar
Prethreshold electron emission to characterize nanostructured objects.
Biomedical Engineering and Nanotechnology Institute, Riga Technical University, Riga, Latvia</td></tr>
<tr><td>11:00-
11:30</td><td colspan="3">Coffee break (Complexo Pedagógico)</td></tr>
<tr><td></td><td>Auditorium 1: Anf. 23.1.7
(Complexo Pedagógico)

Session: New Materials and Advanced Materials
CHAIRS: Prof. Dr. Philip LeDuc, Dr. Gonzalo Guillermo Otero Irurueta</td><td>Auditorium 2: Anf. 22.3.2 (DEM)

Session: Micro / Nano Materials
CHAIRS: Prof. Dr. Yuri Dekhtyar, Dr. Gil Alberto Batista Gonçalves</td><td>Auditorium 3: José Grácio (DEM)

Session: Mechanical Engineering
CHAIRS: Prof. Dr. António Manuel de Bastos Pereira, Prof. Dr. António Manuel Godinho Completo</td></tr>
<tr><td>11:30-
12:00</td><td>Keynote talk
Dr. Dmitry Karpinsky (I16)
Crystal structure of co-doped BiFeO3 ceramics near the phase boundary regions
National Research University of Electronic Technology “MIET”, 124498 Moscow, Russia; Scientific-Practical Materials Research Centre of NAS of Belarus, 220072 Minsk, Belarus</td><td>Keynote talk
Prof. Dr. Salam J.J. Titinchi (O29)
Graphene-Based Porous Adsorbents for CO2 Capture
Department of Chemistry, University of the Western Cape, Cape Town, South Africa</td><td>Keynote talk
Prof. Dr. Ezddin Hutli (I14)
The Relation between the Material Mechanical Properties and the Behaviour in the Fluid-Solid Structures Interaction
Department of Thermohydraulics, Centre for Energy Research, Hungarian Academy of Sciences, Budapest, Hungary; Institute of Nuclear Techniques (INT) of the Budapest University of Technology and Economics (BME), Hungary; Faculty of Mechanical Engineering, Department of Energy Engineering Techniques, Budapest University of Technology and Economics (BME), Hungary</td></tr>
</table>

12:00-12:30	***Keynote talk*** Dr. Indrani Coondoo (**I12**) **An investigation on the impact of the synthesis routes on the electrical properties of lead-free ceramics** *Department of Physics & CICECO, University of Aveiro, Portugal*	***Keynote talk*** Dr. Andrey Kovalskii (**I13**) **Hollow BN spherical nanoparticles: synthesis and applications** *Laboratory of Inorganic Nanomaterials, National University of Science and Technology "MISiS, Leninsky prospect 4, Moscow, 119049, Russian Federation*	**Surface Engineering/Coatings** Ana Antelava (**O25**) **Development of repellent surfaces** *London South Bank University, 103 Borough Rd, London SE1 0AA, United Kingdom*
12:30-14:00	Lunch (UA restaurant)		
14:00-14:45	Auditorium 1: Anf. 23.1.7 (Complexo Pedagógico) Session: **Biomaterials** CHAIRS: Dr. Duncan Paul Fagg, Dr. Igor Bdikin ***Plenary Lecture*** Prof. Dr. Vincent Ball **From prebiotic chemistry to materials science: deposition of aminomalonitrile based films** *Université de Strasbourg. Faculté de Chirurgie Dentaire. 8 rue Sainte Elizabeth. 67000 Strasbourg. France*		
14:45-15:30	Session: **New Methods of Modeling Properties Materials** CHAIRS: Dr. Duncan Paul Fagg, Dr. Igor Bdikin ***Plenary Lecture*** Prof. Dr. Vladimir Bystrov **Modeling of the Piezoelectric and Pyroelectric properties of the ferroelectric composites based on the polyvinylidene fluoride (PVDF) with graphene and graphene oxide layers and fibers** *Inst. Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics RAS, Pushchino, Moscow region, Russia*		
15:30-16:00	Coffee break (Complexo Pedagógico)		
	Auditorium 1: Anf. 23.1.7 (Complexo Pedagógico) Session: **New Materials and Advanced Materials** CHAIRS: Prof. Dr. Salam J.J. Titinchi, Dr. D. Pukazhselvan	Auditorium 2: Anf. 22.3.2 (DEM) Session: **New Methods of Modeling Properties Materials** CHAIRS: Prof. Dr. Herbert Kliem, Prof. Dr. Vladimir Bystrov	Auditorium 3: José Grácio (DEM) Session: **Mechanical Engineering** CHAIRS: Prof. Dr. Vítor António Ferreira da Costa, Prof. Dr. Marco Paulo Soares dos Santos
16:00-16:30	***Keynote talk*** Prof. Dr. Neeraj Panwar (**I11**) **Magnetization reversal and low temperature magnetocaloric effect in rare-**	***Keynote talk*** Dr. José Coutinho (**I4**) **Electronic structure calculations of solids, surfaces and nanostructures.**	**Materials Forming** Olesya Fedchenko (**O14**) **STUDY THE INFLUENCE OF THE PRE-FINISH GAUGES FORM ON THE EFFECTIVENESS OF THE GROOVES FILLING IN THE**

	earth orthochromites: Impact of co-doping *Department of Physics, School of Physical Sciences, Central University of Rajasthan, Bandarsindri-305817, Ajmer, Rajasthan-INDIA*	*I3N & Department of Physics, University of Aveiro, Campus Santiago, 3810-193, Portugal*	**FINISHING PASS OF REINFORCING STEEL ROLLING** *Karaganda state industrial university, 101400, Republic avenue 30, Temirtau, Kazakhstan*
16:30-17:00	Dr. Hanna S. Abbo (**O31**) **Organo functionalised core shell magnetic nanomaterial as adsorbent for aqueous heavy metals removal** *Department of Chemistry, University of Western Cape, Cape Town, South Africa.* *Department of Chemistry, University of Basrah, Iraq*	***Keynote talk*** Dr. Leon Avakyan (**O7**) **Atomic Structure of Multicomponent Metallic Nanoparticles From Extended X-ray Absorption Fine Structure Spectroscopy** *Southern Federal University, Rostov-on-Don, Russia*	**Manufacturing Processes and Mechanical Engineering** Prof. Dr. Boutahari Said (**O22**) **Comparison between linear and nonlinear tolerance analysis of flexible assembly taking into account spot welding effects** *High School of Technology of Fez, University sidi mohamed ben abdellah B.P 2626 –Route d'Imouzzar, 30000 Fez, Morocco*
17:00-17:30	Dr. Dina I. Bakranova (**O4**) **SYNTHESIS OF SILICON CARBIDE FILMS BY MAGNETRON SPUTTERING** *Kazakh-British Technical University, Kazakhstan*	Dr. Budhendra Singh (**O10**) **First Principle study on Structural, Electrical, Optical and Mechanical properties of $GaSe_{1-x}S_x$ solid solution (x = 0,0.25,0.5,0.75,1)** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*	Hafsa ATIK (**O11**) **A new tolerance analysis approach for deformable assemblies: an industrial case study** *High School of Technology of Fez, University sidi mohamed ben abdellah B.P 2626 –Route d'Imouzzar,30000 Fez,Morocco*
17:30-18:00	Monika Nehra (**O38**) **Structural Studies of Metal-Organic Frameworks for Selective Adsorption of Hazardous Contaminants from Aqueous Solutions** *Guru Jambheshwar University of Science and Technology, Hisar-Haryana, 125001, India*	***Keynote talk*** Dr. Ekaterina Paramonova (**O6**) **Magnetic iron substitutions in hydroxyapatite: density functional study** *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, Pushchino, 142290, Russia*	**Low Dimension Structures / Mechanical Engineering** Abdelkadir Belhadj (**O41**) **Free vibration investigation of single walled carbon nanotubes with rotary inertia** *Computational Mechanics Laboratory, Department of Mechanical Engineering, Faculty of Technology, University of Tlemcen, Tlemcen, Algeria*
18:00-18:30	Chimaine FEUDJIO TSAGUE (**O30**) **Surface modification of polyethylenimine coated magnetic nanoparticles in water treatment** *Department of Chemistry, University of the Western Cape, Cape Town, South Africa*		

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<tr><td>9:00-
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CHAIRS: Dr. Duncan Paul Fagg, Dr. Igor Bdikin

Plenary Lecture
Prof. Dr. Nikolai Sobolev
Modification of perpendicular magnetic tunnel junctions by ion irradiation
Physics Department & i3N, University of Aveiro, 3810-193 Aveiro, Portugal; National University of Science and Technology “MISiS”, 119049 Moscow, Russia</td></tr>
<tr><td>9:45-
10:30</td><td colspan="2">Session: New Methods of Modeling Materials Properties
CHAIRS: Dr. Duncan Paul Fagg, Dr. Igor Bdikin

Plenary Lecture
Prof. Dr. Herbert Kliem
A Novel Model for Ferroelectric Imprint in P(VDF-TrFE)
Institute of Electrical Engineering Physics, Saarland University, Building A5 1, 66123 Saabruecken, Germany</td></tr>
<tr><td>10:30-
11:00</td><td colspan="2">Coffee break (Complexo Pedagógico)</td></tr>
<tr><td></td><td>Auditorium 1: Anf. 23.1.7 (Complexo Pedagógico)

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Session: Powder Metallurgy
CHAIRS: Prof. Dr. António Manuel de Bastos Pereira, Prof. Dr. Fernando José Neto da Silva</td></tr>
<tr><td>11:00-
11:30</td><td>Molecular Modelling of Bio-nanostructures
Keynote talk
Prof. Dr. V. S. Bystrov (I2)
Piezoelectric and ferroelectric properties of various amino acids and dipeptides structures: molecular modeling and experiments
Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia</td><td>Keynote talk
Prof. Dr. HAMİT ÖZKAN GÜLSOY (O12)
Influence of Niobium additions on sintering behaviors and mechanical properties of injection molded 420 stainless steel powder
Marmara University, Technology Faculty, Metallurgy and Materials Eng. Dep., 34722 Istanbul, Turkey</td></tr>
</table>

	Composites, Biomaterials	Session: **Nanotechnology**	Auditorium 3: José Grácio (DEM)
11:30-12:00	MOUGHAOUI FATIHA (**O9**) **Removal of Methylene Blue Dye by Adsorption Using Alginate–Clay–Activated Carbon nanobiocomposite** *Biomolecular and Organic Synthesis Laboratory, Faculty of Science Ben M'sik, University Hassan II of Casablanca. Morocco*	Dr. Deepa Kummattummal Govindan (**O18**) **Photocatalytic degradation of methylene blue under visible light using Cu2ZnSnS4 film made of nanoparticle ink** *Interdisciplinary Centre for Energy Research , Department of Instrumentation and Applied Physics, Indian Institute of Science, Bangalore, India*	
12:00-12:30	***Keynote talk*** Prof. Dr. Münir Taşdemir (**O1**) **Mechanical properties of polypropylene bio composites with sea weeds** *Marmara University, Technology Faculty, Metallurgy and Materials Eng. Dep., Istanbul, 34722, Turkey*	Dr. Nimisha Kaippamangalath (**O27**) **Nonlinear Optical and Mechanical Features of Conjugated Polymer Nanocomposites** *Organic Nano Electronic Group, Department of Materials Engineering, Indian Institute of Science Bangalore, India*	
12:30-14:00	Lunch		
	Auditorium 1: Anf. 23.1.7 (Complexo Pedagógico) Session: **Biomaterials** CHAIRS: Prof. Dr. Herbert Kliem, Prof. Dr. Vincent Ball	Auditorium 2: Anf. 22.3.2 (DEM) Session: **Nanotechnology** CHAIRS: Prof. Dr. Nikolai Sobolev, Dr. Gonzalo Guillermo Otero Irurueta	
14:00-14:30	**Biomaterials** ***Keynote talk*** Dr. Pavel Zelenovskii (**I15**) **Chirality-dependent self-assembly of diphenylalanine microtubes** *Department of Physics & CICECO–Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal; School of Natural Sciences and Mathematics, Ural Federal University, 620000 Ekaterinburg, Russia*	Kapil Faliya (**O17**) **Charge Oscillations in PEO from Surface Potential by KPFM** Institute of Electrical Engineering Physics, Saarland University, Germany	
14:30-15:00	Mariia Likhodeeva (**O34**) **DNA-noble metal nanoparticles complexes for biomedical applications** *Saint Petersburg State University, Russia, Saint-Petersburg*	***Keynote talk*** Dr. Olena Okhay (**I9**) **Utilizing reduced graphene oxide for harvesting / storage energy** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*	
15:00-15:30	**Sensor Materials, Biomaterials** Miguel Reis (**O26**) **Thin film functionalization for engineering of biologically active selective sensor surface**	**Low Dimension Structures** ***Keynote talk*** Prof. Dr. Sergey Bozhko (**O36**) **STM lithography at MoO2/Mo(110) surface** *Institute of Solid State Physics RAS, Russia*	

2nd International Conference of TEMA: Mobilizing Projects

	MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Electrical and Computer Engineering, University of Canterbury, Christchurch, 8140, New Zealand		
15:30-16:00	Gul Sirin Ustabasi (**O19**) **Determining the impact of aging on the bacterial toxicity of Zn nanoparticles** *Health Services Vocational School of Higher Education, T. C. Istanbul Aydın University, Sefakoy Kucukcekmece, 34295, Istanbul, Turkey*		
16:00-18:00	**Poster session (Complexo Pedagógico)**		
20:00-22:00	**Conference Dinner**		

12 July 2019

2nd International Conference on Nanomaterials Science and Mechanical Engineering			
	Auditorium 1: Anf. 23.1.7 (Complexo Pedagógico) Session: **Thin Films** CHAIRS: Dr. Duncan Paul Fagg, Dr. Gonzalo Guillermo Otero Irurueta	Auditorium 2: Anf. 22.3.2 (DEM) Session: **Composites** CHAIRS: Dr. Indrani Coondoo, Dr. Gil Alberto Batista Gonçalves	Auditorium 3: José Grácio (DEM)
9:00-9:30	***Keynote talk*** Prof. Dr. Eudes Borges de Araujo (**I1**) **Thermally activated processes and bias field effects on the electrical properties of BiFeO3 thin films** *Department of Physics and Chemistry, São Paulo State University, 15385-000 Ilha Solteira, Brazil*	**Building Materials** Dr. HAMDANE Hasna (**O23**) **Mechanical and microstructural properties of geopolymeric mixtures based on not thermally treated Moroccan phosphate washing sludge: Experimental investigation of new materials as a building materials** *University Hassan II of Casablanca, Faculty of Sciences Ben M'sik. Laboratory of Engineering and Materials. Casablanca, Morocco*	2nd International Conference of TEMA: Mobilizing Projects
9:30-10:00	***Keynote talk*** Dr. Paula Ferreira (**I5**) **Self-standing chitosan-based piezoelectric composite films** *Department of Materials and Ceramic Engineering, CICECO - Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal; TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal*	Younesse HADDAJI (**O20**) **Mechanical and microstructural investigation of Metakaolin/ phosphate washing sludge Based Geopolymers composites Reinforced with polypropylene fibers** *Laboratory of engineering and materials LIMAT, Faculty of science Ben M'Sik, Hassan II University, Casablanca, Morocco*	
10:00-10:30	Coffee break (Complexo Pedagógico)		
	Session: **Thin Films** CHAIRS: Prof. Dr. Eudes Borges de Araujo, Dr. Gonzalo Guillermo Otero Irurueta	Session: **Composites** CHAIRS: Dr. Gil Alberto Batista Gonçalves, Prof. Dr. Paula Alexandrina de Aguiar Pereira Marques	
10:30-11:00	***Keynote talk*** Dr. Oleksandr Tkach (**I8**) **Strain mediated substrate effect on the properties of polar dielectric thin films** *Department of Materials and Ceramic Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, Aveiro, 3810-193, Portugal*	Dr. Maryam Salimian (**O40**) **Synthesis and characterization of Ni/rGO nanocomposite: from nickel nanoclusters to homogeneously distributed discrete nickel nanoparticles** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*	

11:00-11:30	Katarzyna Mituła (**O3**) **Multi(alkenyl)functionalized silsesquioxanes as potential polysiloxanes modifiers** *Adam Mickiewicz University in Poznan, Umultowska 89C, 61-614 Poznan, Poland*	Martina Kocijan (**O28**) **Synthesis of TiO2-rGO nanocomposites as photocatalysts for the degradation of methylene blue dye in water** *Department of Materials, Faculty of Mechanical Engineering and Naval Architecture University of Zagreb, Ivana Lučića 1, 10000 Zagreb, Croatia*	Auditorium 3: José Grácio (DEM)
11:30-12:00	António Fróis (**O5**) **DLC coatings for better orthodontics alloys performance** *CEMMPRE-DEM, Universidade de Coimbra, Pólo II, Rua Luís Reis, 3030-788, Coimbra, Portugal*	Oumaima JAMAL EDDINE (**O8**) **Synthesis and characterization of phosphate glass fibers: mechanical and luminescence properties** *University Hassan II, F. S. Ben M'sik, Laboratory LIMAT, Boulevard Cdt Driss Harti, BP.7955, Ben M'sik - Casablanca - Morocco*	
12:00-12:30		Talha Baig (**O16**) **Synthesis and characterization of gold nanoparticles immobilized on vinyl modified sepiolite** *The City School, Capital Campus, Islamabad, Pakistan*	
12:30-14:00	Lunch		
	Session: **Thin Films** CHAIRS: Dr. Paula Ferreira, Dr. Oleksandr Tkach	Session: **Nanotechnology** CHAIRS: Dr. Isabel Maria Alexandrino Duarte, Prof. Dr. Neeraj Panwar	
14:00-14:30	Dr. Mourad Mebarki (**O13**) **Physical properties of Fe1-xCux films electrodeposited on porous and non-porous silicon** *Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE), 2, Bd Frantz Fanon, BP 140 Alger 7- Merveilles 16038, Algeria*	***Keynote talk*** Dr. Andrei Kovalevsky (**I10**) **Oxide thermoelectrics: redox tuning of the functional properties** *CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal*	
14:30-15:00	***Keynote talk*** Prof. Dr. Sergey Bozhko (**I7**) **Dynamic of molecules rotation in monolayer C60 film.** *Institute of Solid State Physics RAS, Russia*	Dr. Niloufar Raeis-Hosseini (**O37**) **Reconfigurable Metamaterial Perfect Absorber** *Imperial College London, Department of Electrical and Electronic Engineering, South Kensington, London, SW7 2BT, UK*	
15:00-15:30	Prof. Dr. Aleksandr Bagmut (**O21**)	Prof. Dr. Musaab ZAROG (**O35**)	

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	Crystal growth modes and crystallization kinetics of amorphous films according to transmission electron microscopy "in situ" *National Technical University "Kharkiv Polytechnic Institute", NTU "KhPI" 2, Kyrpychova sr., 61002, Kharkiv, Ukraine*	**Sizing Electrode and its effect on performance of a microactuator** *Department of Mechanical and Industrial Engineering, College of Engineering, Sultan Qaboos University, P.O. Box 33, Al-Khod, Muscat, 123, Oman*	Auditorium 3: José Grácio (DEM)
15:30-16:00	Coffee break (Complexo Pedagógico)		
	Session: **Thin Films** CHAIRS: Prof. Dr. Sergey Bozhko, Dr. Duncan Paul Fagg	Session: **Nanotechnology** CHAIRS: Dr. Denis Alikin, Dr. Igor Bdikin	
16:00-16:30	**Low Dimension Structures Laser Processing** Dr. Georgiy Shakhgildyan (**O32**) **Femtosecond laser processing of Ag/CdS doped oxide glasses** *Mendeleev University of Chemical Technology of Russia, 9 Miusskaya sq., Moscow, Russia*	***Keynote talk*** Dr. Maciej Wojtaś (**I3**) **Strong piezoelectricity in Pirydyl-Alanine based hybrid crystals.** *Faculty of Chemistry, University of Wrocław, 14 Joliot-Curie, 50-383 Wrocław, Poland*	
16:30-17:00	**New Energy Materials** ***Keynote talk*** Dr. D. Pukazhselvan (**I6**) **High capacity hydrogen storage: current developments and future perspectives.** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*	Alexander Abramov (**O34**) **Local Electric-Field Induced Phase and Domain Transformations in (1-x)BiFeO3-BaTiO3 systems** *School of Natural Sciences and Mathematics, Ural Federal University, Ekaterinburg, Russia*	
17:00-17:30	**Hydrogen and Fuel Cell Science** Francisco J. A. Loureiro (**O39**) **Proton conductivity in BCY10 in nominally dry conditions** *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*	**Environmental Friendly Materials, Composites** Prof. Dr. Shaista Taimur (**O15**) **Influence of synthesis parameters on polyamidoxime chelating nanohybrid by radiation induced graft polymerization and emulsion graft polymerization for copper (II) uptake** *Balochistan University of Information Technology, Engineering and Management Sciences, Baleli, Quetta, Pakistan; Department of Metallurgy and Materials Engineering, Pakistan Institute of Engineering and Applied Sciences, PO Nilore, Islamabad, Pakistan*	
17:30-18:00	Auditorium 1: Anf. 23.1.7 (Complexo Pedagógico) **Conference Closing Ceremony**		

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Poster session, 16:00-18:00, 11 July

P1	**XPS, FTIR and photoelectron emission spectroscopies to analyze nanocapacitor silicon nitride nano layered structures** Mindaugas Andrulevičius, Liga Avotina, Yuri Dekhtyar, Gennady Enichek, Marina Romanova, Evgeny Shulzinger, Hermanis Sorokins, Sigitas Tamulevičius, Aleksandr Vilken, Aleksandr Zaslavski *Kaunas University of Technology, K. Donelaičio g. 73, Kaunas 44249, Lithuania; University of Latvia, Raiņa blvd 19, LV-1586, Riga, Latvia; Riga Technical University, LV1658, 1 Kalku str, Riga, Latvia; Joint-Stock Company ALFA RPAR, Ropazu str 140, LV-1006, Riga, Latvia*
P2	**Ferroelectric domain wall motion in lead-free BST thin films** M.S. Afanasiev, G.V. Chucheva, D.A. Kiselev Fryazino branch of the Kotel'nikov Institute of Radioengineering and Electronics of *Russian Academy of Sciences, Vvedensky Square 1, Fryazino, Moscow region, Russia; Department of Materials Science of Semiconductors and Dielectrics, NUST "MISiS"*
P3	**Development of magnetic nanoparticles for use in conjunction with radiofrequency heating for greener processes** Duaa Raja, Javier Fernandez Garcia, Ali Hassanpour, Jason Ho *University of Leeds, Leeds, LS2 9JT, UK; South University of Science and Technology of China,1088 Xueyuan Ave, Nanshan, Shenzhen, Guangdong, China*
P4	**Optimizing Citral-loaded Lipid Nanoparticles using a 2^2 Experimental Factorial Design** Zielinska, A., Dias-Ferreira, J., Ferreira, N.R., Silva, A.M., Nowak, I., Souto, E.B. *Faculty of Pharmacy, University of Coimbra, Coimbra, Portugal; Faculty of Chemistry, Adam Mickiewicz University in Poznań, Poland; University of Trás-os-Montes and Alto Douro, Portugal; Centre for Research and Technology of Agro-Environmental and Biological Sciences (CITAB-UTAD); CEB - Centre of Biological Engineering, University of Minho, Campus de Gualtar 4710-057 Braga, Portugal*
P5	**Lipid Nanomaterials for the Targeting of Triamcinolone Acetonide to Retinal Müller Cells in vitro** Dias-Ferreira, J., Zielinska, A., Silva, A. M, Sanchez-Lopez, E., Garcia, M. L., Souto, E. B. *Department of Pharmaceutical Technology, Faculty of Pharmacy, University of Coimbra, Portugal; Department of Faculty of Chemistry, Adam Mickiewicz University in Poznań, Poland; School of Life and Environmental Sciences (ECVA), University of Trás-os-Montes and Alto Douro, Portugal; Centre for Research and Technology of Agro-Environmental and Biological Sciences (CITAB-UTAD), Quinta de Prados; 5001-801 Vila Real, Portugal; Department of Pharmacy, Pharmaceutical Technology and Physical-Chemistry, Faculty of Pharmacy, University of Barcelona, Spain; Institute of Nanoscience and Nanotechnology (IN2UB), Faculty of Pharmacy, University of Barcelona, Spain; CEB - Centre of Biological Engineering, University of Minho, Campus de Gualtar 4710-057 Braga, Portugal*
P6	**Di- and tetrasubstituted double-decker silsesquioxanes as building blocks for molecular and macromolecular frameworks** Julia Duszczak, Beata Dudziec, Michał Dutkiewicz *Faculty of Chemistry, Adam Mickiewicz University in Poznan, Umultowska 89B, 61-614 Poznan, Poland; Centre for Advanced Technologies, Adam Mickiewicz University in Poznan, Umultowska 89c, 61-614 Poznan, Poland; Adam Mickiewicz University Foundation, Rubiez 46, 61-612 Poznan, Poland*
P7	**SYNTHESIS OF NANOSTRUCTURES AND FILMS USING HIGH-TEMPERATURE VACUUM ELECTRIC FURNACE** K.Kh. Nussupov, N.B. Beisenkhanov, S. Keiinbay, D.I. Bakranova, A.A. Turakhun, A.A. Sultan *Kazakh-British Technical University, Kazakhstan*
P8	**The structures of non-IPR isomers 29 (C2), 31 (Cs), 38 (D2) and 39 (D5d) of fullerenes C40** Khamatgalimov A.R., Idrisov R.I., Kamaletdinov I.I., Kovalenko V.I. Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, *Russian Academy of Sciences, 8 Arbuzova str., 420088 Kazan, Russia; Kazan National Research Technological University, 68 K. Marx str., 420015, Kazan, Russia*

P9	**Ythrene: Radical Fullerene Substructure in Fullerenes Molecules** Khamatgalimov A.R., Melle-Franco M., Gaynullina A.A., Kovalenko V.I. Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, *Russian Academy of Sciences, 8 Arbuzova str., 420088 Kazan, Russia; CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 38; 10-193, Aveiro, Portugal; Kazan National Research Technological University, 68 K. Marx str., 420015, Kazan, Russia*
P10	**Titanium oxide-peroxide as a precursor for preparing titania coatings** P.V. Akulinin, A.A. Bezdomnikov, L.N. Obolenskaya, E.V. Savinkina *Lomonosov Institute of Fine Chemical Technology, RTU MIREA, Vernadskogo 86, Moscow, Russia*
P11	**Influence of Structure and Aggregation State of Silver-Gold Nanoparticles on Optical Extinction Spectra** Anna Skidanenko, Leon Avakyan, Maximilian Heinz, Manfred Dubiel, Lusegen Bugaev *Southern Federal University, Department of Physics, Zorge Str. 5, RU-344090 Rostov-on-Don, Russia; Martin Luther University Halle-Wittenberg, Institute of Physics, Von-Danckelmann-Platz 3, D-06120 Halle (Saale), Germany*
P12	**First-principles investigation of structural, magnetic and optoelectronic properties of Mn and Gd doped zinc blende CdS** Hakima HEDJAR, Abdelkader BOUKORTT, Messouda LANTRI, Amel BENYAGOUB *University of Abd ElHamid Ibn Badis-MOSTAGANEM-ALGERIA*
P13	**A new family of alkynylsubstituted silsesquioxanes** Monika Rzonsowska, Kinga Zmudzińska, Beata Dudziec *Faculty of Chemistry, Adam Mickiewicz University in Poznań, Umultowska 89b, 61-614 Poznań, Poland; Centre for Advanced Technologies, Adam Mickiewicz University in Poznań, Umultowska 89c, 61-614 Poznań, Poland*
P14	**Single source precursor synthetic route to quaternary chalcogenide Cu2FeSnS4 nanocrystals as potential solar energy materials** Abdulaziz. M. Alanazi, Firoz Alam, David. J. Lewis, Paul O'Brien *School of Chemistry and Materials, the University of Manchester, Oxford Road UK, M13 9PL; Schools of Materials, the University of Manchester, Oxford Road UK, M13 9PL; School of Chemistry, Islamic university, Prince Naif Ibn Abdulaziz Rd, Madinah, 42351, KSA.*
P15	**Synthesis of maleic anhydride copolymer catalyzed by maghnite-H+** Bettahar Faiza, Bekkar Fadila, Ferahi Mohammed Issam *Polymer Chemistry Laboratory, Department of Chemistry, Faculty of Exact and Applied Science, University of Oran 1. Ahmed Benbella. BP No. 1542 El'Menoeur, 31000 Oran, Algeria.*
P16	**Micro- and nanohardness of gallium sulfide crystals** Elena Borisenko, Nikolai Kolesnikov, Dmitrii Borisenko, Anna Timonina, Budhendra Singh, and Igor Bdikin *Institute of Solid State Physics, the Russian Academy of Sciences, Chernogolovka, Russia; TEMA-NRD, Mechanical Engineering Department, University of Aveiro, 3810-193 Aveiro, Portugal*
P17	**Basal cell carcinoma-targeted therapy using aptamer functionalized liposomes** Anca Niculina Cadinoiu, Delia Mihaela Rață, Leonard Ionuț Atanase, Oana Maria Darabă, Gabriela Vochita, Marcel Popa *"Apollonia" University, Faculty of Medical Dentistry, Pacurari Street, No. 11, Iasi, Romania; Department of Experimental and Applied Biology, Institute of Biological Research Iasi, Lascar Catargi 47, Iasi, Romania; Academy of Romanian Scientists, Plaiul Independentei Street, No 54, Bucharest, Romania*
P18	**Aptamer-Functionalized Polymeric Nanocapsules — a promising alternative for the Basal Cell Carcinoma treatment** Rata Delia Mihaela, Anca Cadinoiu, Leonard Ionut Atanase, Luiza Madalina Gradinaru, Mihai Cosmin-Teodor, Marcel Popa

	Faculty of Dental Medicine, "Apollonia" University of Iasi, Romania; "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania; Institute of Biological Research Iasi, branch of NIRDBS, Iasi, Romania; CEMEX, Grigore T. Popa University of Medicine and Pharmacy Iasi, Romania
P19	**Synthesis and Structural Characterization of Erbium Electrodepositing on Silicon nanowires** A. Brik, S.B.Assiou, T.Hadjersi, B. Benyahia, A. Manseri *Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE)* *2 Bd Frantz Fanon, B.P.140 Alger-7 Merveilles, Algiers (Algeria)*
P20	**Influence of the magnetic field on the structure and properties of epoxy composites with metal oxides** Yuliia Bardadym, Edward Sporyagin, Oleksandr Naumenko *Institute of Macromolecular Chemistry of NAS of Ukraine; Oles Honchar Dnipro National University; Ukrainian State University of Chemical Technology*
P21	**Minimization of the concentration quenching effect of Tris(bipyridine)ruthenium(II) chloride dye** Olga Lu, Akbota Yensebayeva, Irina Irgibaeva, Artur Mantel *L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*
P22	**Silicon nanowires modified by nanocomposites materials-based graphene oxide for enhanced photodegradation of organic dye** Naama Sabrina, Benkara Amira, Khen Adel, Baba Ahmed Latifa, Hadjersi Toufik, Manseri Amar *Research Center in Semiconductors Technology for Energetic (CRTSE). 2, Bd. Frantz Fanon, B.P. 140 Alger-7 Merveilles, Algiers, Algeria; University of Saad Dahleb Blida 1,street of Soumaa, BP 270, Blida 09000, Algeria*
P23	**Electrochemical contribution to local electromechanical response in P(VDF-TrFe)/LiNbO3** Maxim V. Silibin , Maxim S. Ivanov, Vladimir A. Khomchenko, Timur Nikitin, Arseny S. Kalinin, Dmitry V. Karpinsky, Vyacheslav V. Polyakov, Rui Fausto and Jose A. Paixão *National Research University of Electronic Technology "MIET," Zelenograd, 124498 Moscow, Russia; CFisUC, Department of Physics, University of Coimbra, 3004-516 Coimbra, Portugal; CQC, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal; NTMDT Spectrum Instruments, Zelenograd, 124460 Moscow, Russia*
P24	**Facile wet chemical powders synthesis for Copper Oxide thin films preparation and gas sensing applications** S. BOUACHMA, Z. BOUKHEMIKHEM, A. MANSERI, N. GABOUZE *Semiconductor Technology Research Center for Energetics: Ave Doctor Frantz Fanon BP 140, Algiers, Algeria*
P25	**Structural properties of silicone carbide nanoparticles produced by sol-gel method** Karima Benfadel, Samira Kaci, Fahim Hamidouche, Aissa Keffous, Abdelbaki Benmounah *CMSI, Semiconductor Technology Research Center for Energetics, (CRTSE), 2UR-MPE: research unit materials, processes and environment M'hamed Bougara University.*
P26	**Ti surface nanoarhitecturing for gliadin identification** Dumitriu Cristina, Pirvu Cristian *University Polytechnic of Bucharest, Faculty of Applied Chemistry and Materials Science, 1-7 Polizu, 011061, Bucharest, Romania*
P27	**Physicochemistry of Hyaluronic-based Oil Core Nanocapsules for Drug Delivery** Małgorzata Janik, Justyna Bednorz, Joanna Szafraniec, Szczepan Zapotoczny *Jagiellonian University, Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry, Gronostajowa 2 30-387 Cracow, Poland; Jagiellonian University Medical College, Faculty of Pharmacy, Department of Pharmaceutical Technology and Biopharmaceutics, Medyczna 9 30-688 Cracow, Poland.*
P28	**Nano- and microstructures formed from hydrophobic homopolymer and amphiphilic copolymer – comparative study** Maria Zatorska, Urszula Kwolek, Natalia Wilkosz, Aleksandra Urych, Keita Nakai, Dorota Jamróz, Shin-ichi Yusa, Mariusz Kępczyński

	Jagiellonian University, Faculty of Chemistry, 2 Gronostajowa St., 30-387 Cracow, Poland; University of Hyogo, Graduate School of Engineering, Department of Materials Science and Chemistry, 2167 Shosha Himeji, Hyogo 671-2280, Japan.
P29	**Interactions of Polycations with Anionic Lipid Membranes** Agata Żak, Kinga Liczmańska, Rina Nakahata, Shin-ichi Yusa, Mariusz Kępczyński *Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387 Kraków, Poland; University of Hyogo, Department of Applied Chemistry, 2167 Shosha, Himeji, Hyogo 671-2280, Japan.*
P30	**Intercalation of magnetic nanoparticles into bitumen** Kurmetkhan Sanzhar, Issayeva Amina, Irina Irgibaeva, Artur Mantel, Mendigalyeva Svetlana *L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*
P31	**Influence of ions-releasing surfaces on grafting of polymer brushes** Gabriela Grześ, Karol Wolski, Anna Gruszkiewicz, Joanna Rokita, Szczepan Zapotoczny *Jagiellonian University, Faculty of Chemistry, Department of Physical Chemistry and Electrochemistry, Gronostajowa 2, 30-387 Cracow, Poland*
P32	**Luminescent properties of novel Ce-doped ZnO:SiO2 nanosized films under the action of bovine myoglobin** Hayrullina I., Nagovitsyn I.A., Sheshko T.F., Chudinova G.K., Boruleva E.A. *Peoples' Friendship University of Russia (RUDN University), 6 Miklukho-Maklaya Str., Moscow, 117198, Russia Federation; General Physics Institute RAS, 38 Vavilov Str., Moscow, 119991, Russia Federation; Semenov Institute of Chemical Physics RAS, 4 Kosygina Str., Building 1, Moscow, 119991, Russian Federation; National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoye shosse, Moscow, 115409, Russia Federation*
P33	**A green Functionalization of Poly(ethylene glycol) for Use as biomaterials** Sara HAOUE, Mohammed BELBACHIR *Laboratory of Polymer Chemistry, Department of Chemistry, Faculty of Sciences, University Ahmed Ben Bella Oran, BP 1524,ElM'nouar 31000 Oran, Algeria*
P34	**Synthesis and characterization of TEOS/VES silicone nanoparticles** R. Petka, A. Łatkiewicz, O. Woznicka, M. Romek, M. Kepczynski *Faculty of Chemistry, Jagiellonian University, 2 Gronostajowa, 30-387 Kraków, Poland; Institute of Geological Sciences, Jagiellonian University, 3a Gronostajowa, 30-387 Kraków, Poland; Institute of Zoology, Jagiellonian University, 9 Gronostajowa, 30-387 Kraków, Poland*
P35	**Structural Study of Silicon nitride thins films doped with Cerium** K. Bekhedda, A. Brik, B. Benyahia, H. Menari, A. Manseri *Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE)* *2 Bd Frantz Fanon, B.P.140 Alger-7 Merveilles, Algiers (Algeria).*
P36	**Porous silicon double membranes for lithium- ion batteries** C. Yaddaden, A. Cheriet, M. Berouaken and N. Gabouze *Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE), 02 Bd, Frantz Fanon, B.P. 140, Algiers, Algeria.*
P37	**MODIFICATIONS ON THE CRYSTALLINE STRAIN AND SIZE IN THE PHASE FORMATION OF MULTIFERROIC BISMUTH FERRITE NANOPARTICLES** Venkatapathy Ramasamy, Yathavan Subramanian, Durairajan Arulmozhi, Manuel Pedro Fernandes Graca, Manuel Almeida Valente, Gokulraj Srinivasan and Ramesh Kumar Gubendiran *Department of Physics / University College of Engineering Arni, Anna University, India;* *I3N-Aveiro-Department of Physics / University of Aveiro, Portugal; Department of Physics / C. Kandasamy Naidu College for Men Chennai. India*
P38	**Swift Heavy Ion Irradiation effect on Ferroelectric Triglycine Sulphate (TGS) Single Crystals** V.C. Bharath Sabarish, A. Durairajan, G. Ramesh Kumar,M. P. F. Graca, M. A. Velente, E. V. Ramana, S. Gokulraj

	Departement of Physics, University College of Engineering Arni -Thatchur 632 326, India; 3N-Aveiro, Department of Physics, University of Aveiro, Aveiro 3810 193, Portugal; Department of Physics,C.Kandasamy Naidu College for Men Chennai, India.
P39	**Two spectral infrared detectors based on HgCdTe epitaxial layers** K. Andrieieva, F. Sizov, Z. Tsybrii, M. Vuichyk, M. Apatska, S. Bunchuk, N. Dmytruk, M. Smolii, I. Lysuk, K. Svezhentsova *V.E. Lashkaryov Institute of Semiconductor Physics, 41 pr. Nauky, Kyiv, Ukraine*
P40	**The synthesis and characterization of a new class of conductive polymers** Bekkar Fadila, Bettahar Faiza, Meghabar Rachide Hammadouche Mohammed Belbachir. *Laboratory of Polymer Chemistry, Department of Chemistry, Faculty of Science, University Oran1 Ahmed Ben bella. BP N°1524 El'Menouer, 31000 Oran, Algeria; Laboratory of Fine Chemistry, Department of Chemistry, Faculty of Science, University Oran1 Ahmed Benbella. BP N°1524 El'Menouer, 31000 Oran, Algeria.*
P41	**Esterification of polyvinyl alcohol with abietic acid in the presence of a green Maghnite-H+ ctalyzer** Badia Imene Cherifi, Mohammed Belbachir *Laboratory of Polymer Chemistry, Department of Chemistry, Faculty of Exact and Applied Sciences, University Oran 1 Ahmed Ben Bella, BP 1524 El M'Naouar, 31000Oran, Algeria*
P42	**Synthesis of 1D and 2D ZnO/Ag/CdS nanocomposites to photon driven hydrogen production** Bakranov N., Kudaibergenov S. *Kazakh National Research Technical University after K.I.Satpayev, Satpayev street. 22, Almaty, Kazakhstan; Institute of Polymer Materials and Technologies, Microdistrict Atyrau-1, 3/1, Almaty, Kazakhstan.*
P43	**Growth and spectral characteristics of KY(WO4)2 : Ho3+ single crystals** S. Guretsky, D. Karpinsky, I. Kolesova, A. Kravtsov, O. Dernovich, S. Özçelik, N. Kuleshov *Scientific and Practical Materials Research Center NAS Belarus, Minsk, Belarus; Belarusian National Technical University, Minsk, Belarus; Photonics Application and Research Center, Gazi University, Ankara, Turkey*
P44	**Structural Properties of Sol-Gel BiFeO3- Films** S.A. Khakhomov, V.E. Gaishun, D.L. Kovalenko, A.V. Semchenko, V.V. Sidsky, O.I. Tyelenkova, W. Strek, D. Hreniak, A.L. Kholkin, S. Kopyl, I. Bdikin *F. Skorina Gomel State University, Sovetskaya 104, Gomel, 246019, Belarus; Institute of Low Temperature and Structures Research PAN, Okolna st. 2, Wroclaw, Poland; University of Aveiro, Campus Universitário de Santiago, Aveiro, 3810-193, Portugal*
P45	**Investigation of Bi0,9La0,1FeO3 Sol-Gel films by XRD** S.A. Khakhomov, V.E. Gaishun, D.L. Kovalenko, A.V. Semchenko, V.V. Sidsky, W. Strek, D. Hreniak, A.L. Kholkin, S. Kopyl, I. Bdikin, O. V. Ignatenko *F. Skorina Gomel State University, Sovetskaya 104, Gomel, 246019, Belarus; Institute of Low Temperature and Structures Research PAN, Okolna st. 2, Wroclaw, Poland; University of Aveiro, Campus Universitário de Santiago, Aveiro, 3810-193, Portugal; Scientific-Practical Materials Research Centre of National Academy of Sciences of Belarus, P.Brovki st. 19, Minsk, 220072, Belarus*
P46	**Synthesis of BiFeO3 and Bi0,9Sm0,1FeO3 films by Sol-Gel method** S.A. Khakhomov, V.E. Gaishun, D.L. Kovalenko, A.V. Semchenko, V.V. Sidsky, V.V. Vaskevich, A.N. Aleshkevich, A.L. Kholkin, S. Kopyl, I. Bdikin, A. Kareiva, Z. Stankeviciute *F. Skorina Gomel State University, Sovetskaya 104, Gomel, 246019, Belarus; Institute of Low Temperature and Structures Research PAN, Okolna st. 2, Wroclaw, Poland; University of Aveiro, Campus Universitário de Santiago, Aveiro, 3810-193, Portugal; Vilnus University, Universiteto g. 3 Vilnius, 01513, Lithuania.*
P47	**Modification of interface-controlled parameters of magnetic tunnel junctions by ion irradiation** B. M. S. Teixeira, A. A. Timopheev, N. F. F. Caçoilo, J. Mondaud, J. R. Childress, E. Alves, N. A. Sobolev *Physics Department & i3N, University of Aveiro, 3810-193 Aveiro, Portugal; Crocus Technology, 3 avenue Doyen Louis Weil, BP1505 - 38025 GRENOBLE Cedex1, France; IPFN, Instituto Superior Técnico,*

	Universidade de Lisboa, 2695-066 Bobadela LRS, Portugal; National University of Science and Technology "MISiS", 119049 Moscow, Russia
P48	**Conjugation of nanomaterials in cellulose filter paper for superior water filtration** Sandeep Kumar, Monika Nehra, Shikha Jain, Neeraj Dilbaghi, Ki-Hyun Kim *Department of Bio and Nano Technology, Guru Jambheshwar University of Science and Technology, Hisar-Haryana, 125001, India; Department of Electronics and Communication Engineering, Guru Jambheshwar University of Science and Technology, Hisar- Haryana, 125001, India; Department of Civil & Environmental Engineering, Hanyang University, 222 Wangsimni-Ro, Seoul 04763, Republic of Korea*
P49	**Polarization and Piezoelectric properties of ZnO nanoparticles/nanorods interacting with various dopant and PVDF structures: molecular modeling and experiments** V. S. Bystrov, I. K. Bdikin, B. Singh, B.Kumar *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; Crystal Lab, Department of Physics & Astrophysics, University of Delhi, Delhi-110007, India*
P50	**Properties optimization by Al doping of ZnMgO for transparent conductive oxide (TCO) films** Amel Bahfir, Messaoud Boumaour, Mouhamed Kechouane, Hadjira Labech *Research Center in Semiconductors Technology for Energetic (CRTSE). 2, Bd. Frantz Fanon, B.P. 140 Alger-7 Merveilles, Algiers, Algeria; University of science and Houari Boumediene- USTHB - Bab-Ezzouar, Algiers, Algeria*
P51	**Li vacancies effect onto Li/Si alloys properties: theoretical investigation** A. LARABI, M. MEBARKI, A. Mahmoudi and N. Gabouze (61) *Centre de Recherche en Technologie des Semi-conducteurs pour l'Energétique (CRTSE), 2, Bd Frantz Fanon, BP 140 Alger 7- Merveilles 16038, Algerie*
P52	**Local piezoelectric properties of dipeptide nanotube structures** Budhendra Singh, V.S. Bystrov, Nuno Almeida, I.K. Bdikin *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal; Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia*
P53	**Development of new materials for air purification applications** Maryam Salimian, Nuno A. F. Almeida, Eduarda B. H. Santos and Paula A. A. P. Marques *TEMA, Department of Mechanical Engineering, University of Aveiro, Portugal*
P54	**TiO2-rGO nanocomposite immobilized in P(VDF-TrFE): a sunlight active and reusable photo-catalyst for the elimination of metoprolol in water** Silva V., Salimian M., Marques P. A. A. P., Santos E. B. H. *Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal, valentinagsilva@ua.pt and telephone: +351916198762; TEMA, Department of mechanical engineering, University of Aveiro, 3810-193 Aveiro, Portugal; CESAM, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal.*
P55	**Modeling of dichalcogenide MoS2 monolayers and its composites with PVDF/P(VDF-TrFE)** V. S. Bystrov, Hong Shen, Xiangjian Meng *Institute of Mathematical Problems of Biology, Keldysh Institute of Applied Mathematics, RAS, 142290 Pushchino, Moscow region, Russia; Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai 200083, China*
P56	**Mechanical properties and fracture mechanism of Ti3Al intermetallic produced by powder metallurgy and casting processes** D. Božić, B. Dimčić, J. Stašić *University of Belgrade, Mike Petrovića Alasa 12-14, P.O. Box 522, 11001 Belgrade, Serbia*
P57	**The effect of picosecond laser on silver target – surface modification and nanoparticles production** J. Stašić, M. Trtica *University of Belgrade, Mike Petrovića Alasa 12-14, P.O. Box 522, 11001 Belgrade, Serbia*

P58	**Comparison of surface topography in machining Ti alloys for biomedical applications: Correlative microscopy approach for qualitative and quantitative analysis** Sílvia Carvalho, Ana Horovistiz, A. J. Festas, J.P. Davim *TEMA, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal*
P59	**A comparative study between conventional drilling and helical milling in titanium alloys for medical applications** A. J. Festas, R. B. Pereira, A. Ramos, J. P. Davim *Dep. of Mechanical Engineering, University of Aveiro, Campus Santiago, 3010-193 Aveiro, Portugal; Dep. of Mechanical Engineering, Federal University of São João Del-Rei, 170 Frei Orlando Square, São João Del-Rei, MG 36880-000, Brazil.*
P60	**Sintering Atmosphere Effect on Powder Injection molded AISI-420 stainless steel powder** Lutfi Yakut, H.Ozkan Gulsoy *Marmara University, Inst. Graduate Studies Pure and Applied Sci., 34722, Istanbul, Turkey; Marmara University, Technology Faculty, Metallurgy and Materials Eng. Dep., 34722 Istanbul, Turkey*
P61	**A biomimetic engineered texture that turns wetting materials omniphobic even under immersion** Eddy M. Domingues, Sankara Arunachalam, Ratul Das, Jamilya Nauruzbayeva and Himanshu Mishra *University of Aveiro, Department of Mechanical Engineering, Centre for Mechanical Technology and Automation, Nanoengineering Research Group; King Abdullah University of Science and Technology, Water Desalination and Reuse Center, Biological and Environmental Science and Engineering Division, Thuwal 23955-6900, Saudi Arabia*
P62	**Growth, structure and magnetic properties of $NdFeO_3$ single crystals** A.Durairajana, E. Venkata Ramana, G. Ramesh Kumar, M.P.F. Graça, M.A. Valente *I3N-Aveiro, Department of Physics, University of Aveiro, Aveiro 3810 193, Portugal; Department of Physics, University College of Engineering Arni, Anna University, India*
P63	**Unusual magnetic properties of BLFO - KBr nanocomposites** Olena M. Fesenko, Andrii Yaremkevich, Dmitry V. Karpinsky, Maxim V. Silibin, Vladimir V. Shvartsman, and Anna N. Morozovska *Institute of Physics, NAS of Ukraine, 46, pr. Nauky, 03028 Kyiv, Ukraine; Scientific-Practical Materials Research Centre of NAS of Belarus, 220072 Minsk, Belarus; National Research University of Electronic Technology "MIET", 124498 Moscow, Russia; Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 45141, Essen, Germany*
P64	**Graphoepitaxial growth of CeO2 thin films on tilted-axes NdGaO3 substrates** Peter B. Mozhaev, Julia E. Mozhaeva, Igor K. Bdikin, Iosif M. Kotelyanskii, Valery A. Luzanov, Jørn Bindslev Hansen, Claus S. Jacobsen *Institute of Physics and Technology of the Russian Academy of Sciences, Moscow, 117218, Russia; TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, Aveiro, 3810-193, Portugal; Kotelnikov Institute of Radioengineering and Electronics of Russian Academy of Sciences, Moscow, 125009, Russia; Department of Physics, Technical University of Denmark, Kongens Lyngby, DK-2800, Denmark*
P65	**Theoretical investigation of structural, electronic and mechanical properties of Al-doped c-BN compound** Budhendra Singh, Igor Bdikin *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, 3810-193, Aveiro, Portugal*
P66	**DFT investigation of mechanical strength of graphene and adsorption of H2 , NO and CO on monolayer graphene and graphene oxide** Budhendra Singh, Igor Bdikin *TEMA-NRD, Mechanical Engineering Department and Aveiro Institute of Nanotechnology (AIN), University of Aveiro, 3810-193, Aveiro, Portugal*
P67	**Synthesis and characterization of Double Pervoskites Halides** Janaradhan Rao, Nitu Salunke, Sonam Unde,Tejaswini Manolikar, Nazia Tarranum, Ranjit Hawaldar

	Centre for Materials for Electronics Technology, Pune, India; Department of Chemistry, Chaudhary Charan Singh University, Meerut, India
P68	**Radiation-induced point defects transformation in irradiated lithium fluoride crystals after their mechanical fragmentation** A. P. Voitovich, V. S. Kalinov, A. N. Novikov, L. P. Runets *B. I. Stepanov Institute of Physics of the National Academy of Sciences of Belarus, 68-2 Nezavisimosti ave., Minsk, 220072, Belarus*
P69	**Development of 3D electrospun PCL/Chitosan scaffolds for musculoskeletal tissue engineering** Andreia Leal Pereira, André F. Girão, Ângela Semitela, Samuel Guieu, Paula A.A.P. Marques, Maria Helena V. Fernandes *CICECO - Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, 3810-193 Aveiro, Portugal; TEMA – Centre for mechanical technology and automation, Department of Mechanical Engineering, University of Aveiro, 3810-193 Aveiro, Portugal; QOPNA & LAQV-REQUIMTE, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal; The Discoveries Centre for Regenerative and Precision Medicine, Headquarters at University of Minho, Avepark, 4805-017 Barco, Guimarães, Portugal*

Plenary Lectures

Planes, Trains, Automobiles....and Cells?

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Two areas that have always interested me are the mechanics of machines and the wonders of nature. My interest in mechanics, first beginning as a youth taking apart machines like lawn mowers, has intersected with my fascination with nature at the cellular and molecular levels. Here I will present how my lab has been merging mechanical engineering with biology. My lab approaches this intersection by envisioning cells and molecules as "systems" that can be investigated with some of the same fundamental approaches used on machines such as planes, trains, and automobiles looking for unifying principles. The biological systems range from mammalian cells to microorganisms to developmental biology systems (e.g. neurons, magnetic bacteria, energy generating bacteria, *Xenopus laevis*, stem cells) and we apply principles from mechanical engineering fields (e.g. solid mechanics, control theory, fluidics, heat transfer, design) to understand how these principles may apply across diverse nature-based systems. In addition, I will present in this talk our approaches of using solid mechanics in areas such as cell mechanotransduction. We pursue these goals through developing and utilizing unique custom-built systems as well as nanotechnology, microtechnology, and computational biology. These intersections are especially fascinating to me as biological systems have evolved for distinct reasons (the "initial and boundary conditions" are different). In addition, as an engineer, I truly am interested in building new systems from the knowledge that we obtain in a similar thought process as we use information to build new machines. Thus, I will also present how our lab thinks about nature-inspired design principles at the molecular and cellular levels to work toward generating novel approaches for contributing to technology development and medical applications. My goal for this talk is to present some of our work and thoughts about how one mechanical engineer approaches these nature-based systems at the cellular and molecular levels.

Prethreshold electron emission to characterize nanostructured objects

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Rapid development of nanomaterials opens a wide horizon for their applications. Reliable employment of materials requires trustworthy detection of their properties. To do not disturb gentle nanoobjects, measurements of them due to contact less technique are very preferable.

The purpose of the rep[ort is to introduce a low energy electron prethreshold (energy of the emitting electron is close to the electron work function) emission to characterize nanostructured objects. Emitting electrons have a mean free path in a solid that is in order of nanoscale. Therefore, a prethreshold electron emission contact less spectroscopy could become a good instrument both for characterization of nanostructured materials and nanosensing. Weak emission (~10^{-16}… 10^{-15} Q/cm^2) of electrons from an emitter does not influence significantly the measured object – its surface electrical charge density that is around 10^{14} cm^{-2} is influenced negligibly.

The paper reviews photo-, dual- and exo- electron emission fundamentals and their applications towards characterization of nanoobjects: concentration of point like imperfections, their annealing, migration; surface charge of nanoparticles; energy gap; electron density of states; thickness of thin films and interfaces between them and the substrate.

The achieved results demonstrate that the prethreshold electron emission spectroscopy is suitable to characterize nanoobjects for different applications: electronics, dosimetry, biomaterials, chemical sensing.

Modeling of the Piezoelectric and Pyroelectric properties of the ferroelectric composites based on the polyvinylidene fluoride (PVDF) with graphene and graphene oxide layers and fibers

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Recent results in modelling and computational studies of new composite nanomaterials based on polymer ferroelectrics and graphene/graphene oxide structures are reviewed. Main findings of the computational molecular modelling and calculations of the plane layered and fibers nanostructures, as well as multi-layered structures, and the piezoelectric and pyroelectric properties of the composites, consisting of polyvinylidene fluoride (PVDF) thin films and graphene/graphene oxide are analysed [1-7]. The piezoelectric and pyroelectric effects were modelled, both piezo- and pyro-electric coefficients were calculated for several models, using various methods from HyperChem software tool, including molecular dynamics (MD) simulation with quantum-chemical semi-empirical PM3 method [5-7].

The data obtained show that the values of the pyroelectric coefficients computed by the MD run method proposed are very close to experimental data and published data [5-7]. Models developed for PVDF/Graphene oxide composites were considered and their piezoelectric coefficients computed by the calculation algorithms described in [3, 4] are discussed in comparison with experimental results [1, 2, 7]. The piezoelectric coefficients d_{33} calculated also for different types of structures of Graphene Oxide with OH and COOH groups and PVDF: for flat layer models and for curved fiber models [2-7].The electromechanical properties of the PVDF/G and PVDF/GO nanofibers, which were investigated by various methods, are discussed. Experimentally measured results qualitatively correlate with the data computed

The results obtained provide important insights into our understanding of the mechanisms of piezoelectricity and pyroelectricity in these new nanocomposites, give us new perspectives for further studies of the ferroelectric polymer–graphene nanomaterials. Authors wish to acknowledge the Russian Foundation for Basic Researches (RFBR) grants # 16-51-53017, # 19-01-00519 A, to the Russian Science Foundation (RSF grant # 16-19-10112) and to the National Natural Science Foundation of China (NNSFC) for grant number # 61574151.

References

[1] V.S. Bystrov, I.K. Bdikin, M.V. Silibin, D.V. Karpinsky, *et al.*, *Ferroelectrics*, 509, 124-142 (2017).
[2] M.V. Silibin, V.S. Bystrov, D.V. Karpinsky, *et al., Applied Surface Science*, 421, Pt A, 42-51 (2017).
[3] V.S. Bystrov, E.V. Paramonova, I.K. Bdikin, *et al., J. Mol. Model.*, 19, 3591–3602 (2013).
[4] V.S. Bystrov, I.K. Bdikin, M. Silibin, *et al., J. Mol. Mod.*, 23, 128 (2017).
[5] V.S. Bystrov, I.K. Bdikin, M. Silibin, X.J. Meng, *et al., J. Phys.: Conf. Series*, 1053, 012043 (2018).
[6] V.S. Bystrov, *et al., Ferroelectrics*, (2019). - https://doi.org/10.1080/00150193.2019.1574637
[7] V.S. Bystrov, In book: Global Conference on Carbon Nanotubes and Graphene Technologies. - Milan, March 28-29, 2019, Italy. - https://scientificfederation.com/graphene-technology-2019/index.php. - p. 15.

Modification of perpendicular magnetic tunnel junctions by ion irradiation

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In this talk, we'll give a short overview over 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 with an easy-cone anisotropy, as well as of complete MTJs comprising the typical Ta / FeCoB / MgO free layer.

In the first part of the study, we irradiated MgO / FeCoB(t_{FCB} / MgO free layers, with and without a 0.2-nm-thick W or Ta spacer, and t_{FCB} = 3.0 nm or t_{FCB} = 2.6 nm, with 400 keV Ar^+ ions at fluences ranging from 10^{12} cm^{-2} to 10^{16} cm^{-2}. B_{K1eff} decreased linearly with the logarithm of the fluence from 10^{12} cm^{-2} to 10^{15} cm^{-2} due to the ion-induced intermixing at the FeCoB / MgO interface. Due to the decrease in PMA caused by the ion irradiation, spin reorientations were induced in these free layers. We effectively produced easy-cone anisotropy, with different cone angles, in 2.6-nm-thick FeCoB layer with a W spacer and obtained a complete spin reorientation from easy axis to easy cone and then to easy plane in the case of the layer with a Ta spacer. Importantly, the irradiation, at fluences for which these transitions occurred, did not increase the Gilbert damping parameter, which is vital, from the application viewpoint, to keep a low current density for STT-switching.

To assess the impact of ion irradiation on the other interface-controlled parameters relevant to pMTJ technology, we irradiated a complete MTJ multilayer with 400 keV Ar^+ ions at fluences up to 5×10^{15} cm^{-2}. The stack was comprised of Substrate / Ta / CuN / Ta / Ru / IrMn / PL / Ru / RL / MgO / FL / Ta/Ru layers, where PL, RL and FL are the pinned, reference and free layers made of CoFe(B) alloys.

The anisotropy keeping the magnetization in-plane decreased with increasing fluence. This tendency, opposite to the observed in MgO / FeCoB / MgO, is explained by a stronger decrease of M_S, due to intermixing at the top FL / Ta interface, than of k_{s1} at the MgO/FL interface.

The TMR dropped from 193% to 74% at 3×10^{13} cm^{-2}, following the decrease in R_{AP}. The intermixing at MgO / FeCoB cannot explain this initial loss of TMR, since B_{K1eff} and R_P

remain practically unchanged up to 3×10^{13} cm^{-2}. The likely mechanism is instead the creation of defects within the MgO barrier, acting as spin-independent tunneling channels shunting the spin-dependent one. Above 10^{14} cm^{-2}, the RL became decoupled from the PL, as seen by the two loops in R(H) and the appearance of an additional FMR line.

Other effects of the irradiation, particularly those concerning the magnetic damping and interlayer couplings, will also be addressed.

References

[1] C. Chappert, H. Bernas, J. Ferré, V. Kottler, J.-P. Jamet, Y. Chen, E. Cambril, T. Devolver, F. Rousseaux, V. Mathet, and H. Launois, Science 280 (1998) 1919.
[2] B. Dieny, and M. Chshiev, Rev. Modern Phys. 89 (2017) 025008.
[3] S. Ikeda, K. Miura, H. Yamamoto, K. Mizunuma, H.D. Gan, M. Endo, S. Kanai, J. Hayakawa, F. Matsukura, and H. Ohno, Nature Mater. 9 (2010) 721.
[4] N. Strelkov, A. Timopheev, R.C. Sousa, M. Chshiev, L.D. Buda-Prejbeanu, and B. Dieny, Phys. Rev. B 95 (2017) 184409.
[5] B.M.S. Teixeira, A.A. Timopheev, N.F.F. Caçoilo, S. Auffret, R.C. Sousa, B. Dieny, E. Alves, and N.A. Sobolev, Appl. Phys. Lett. 112 (2018) 202403.

A Novel Model for Ferroelectric Imprint in P(VDF-TrFE)

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Imprint denotes a reversible time dependent change of ferroelectric material properties. Switching P(VDF-TrFE) to the remanent polarization state P_r at field E_a=0 and waiting in this state for a time t_w yields: (I) an increase of the coercive field, (II) an increase of the switching time τ , (III) a decrease of the small signal ac capacitance while waiting in P_r and (IV) a long lasting decay of $P_r(t_w)$ [1]. The effects are independent of the sample thickness. All four effects exhibit a linear behavior on a logarithmic time scale, i.e. they are proportional to $\log(t_w)$. The four effects are the stronger the bigger the portion of the amorphous phase is. The following model can explain the imprint. In the material, crystals with ferroelectric properties are embedded in an amorphous phase with relaxational dielectric properties. After a switching event the ferroelectric crystals get their stable polarization which generates in the amorphous phase a stray field in antiparallel direction, Fig.1. This stray field aligns the dipoles of the amorphous phase gradually with a

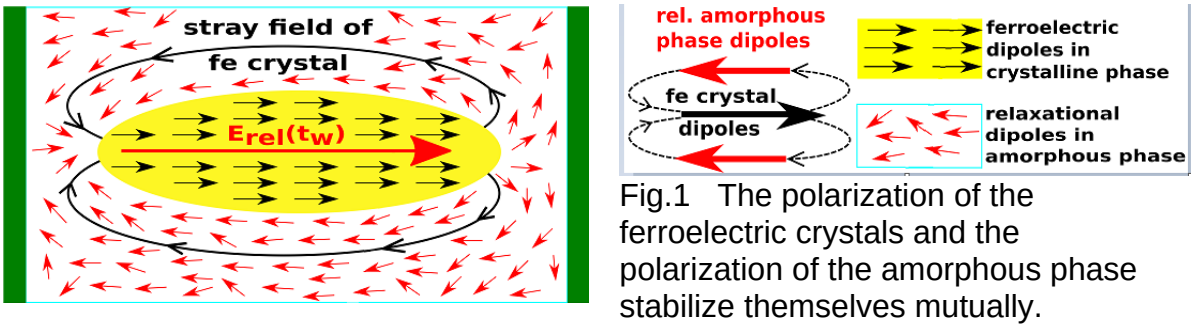

Fig.1 The polarization of the ferroelectric crystals and the polarization of the amorphous phase stabilize themselves mutually.

logarithmic time behavior, because a distribution of relaxation times exists due to the amorphous structure. When these dipoles line up they decrease the total polarization $P_r(t_w)$ of the sample. Vice versa the relaxational dipoles evoke a field $E_{rel}(t_w)$ in the ferroelectric crystals in direction of the ferroelectric polarization which stabilizes the ferroelectric state. This corresponds to two dipoles which align in antiparallel position. The stabilization of the ferroelectric polarization results in an increased field E_c and an increased switching time τ. The decrease of the small signal ac capacitance at E_a=0 results from the shift of the complete hysteresis loop along the field axis. An extended Weiss field calculation can describe the experimental observations [2].

[1] C. Peter, A. Leschhorn, H. Kliem, J. Appl. Phys. **120**, 124105 (2016)
[2] C. Peter, H. Kliem, accepted by J. Appl. Phys.

From prebiotic chemistry to materials science: deposition of aminomalonitrile based films

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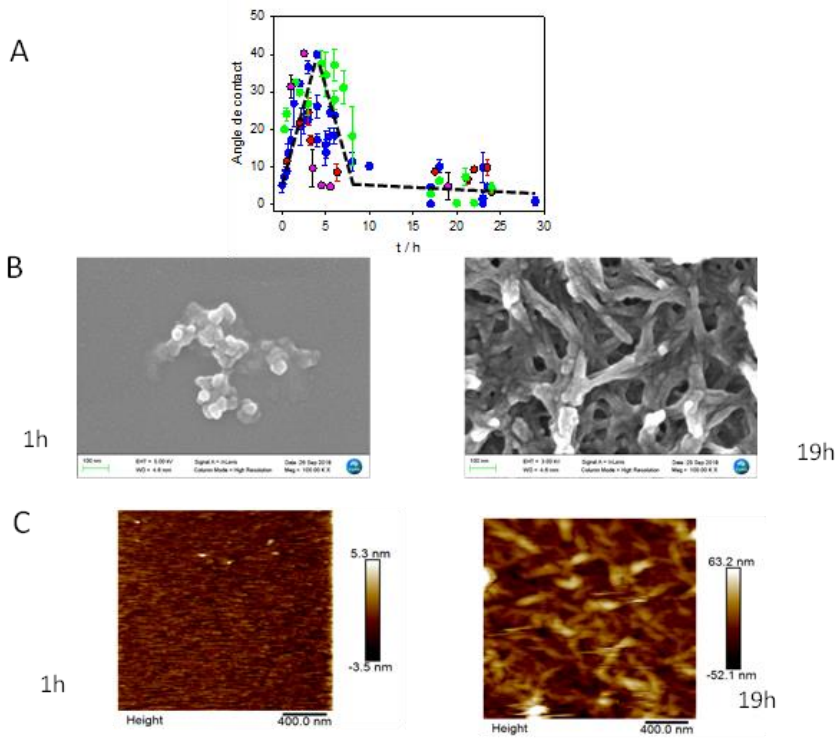
Surface functionalization with strongly adhesive and easy to functionalyze films has remained highly materials specific for a long time. But bioinspiration from the mussel which is able to adhere to almost all known materials under wet conditions has allowed the development of polydopamine films from the oxidation of dopamine [1]. Other molecules seem promising in this perspective: inspiration from prebiotic chemistry and from the famous experience realized by prof. Miller [2] allowed to demonstrate that strongly adhesive and biocompatible films can be deposited at solid-liquid interfaces from aminomalonitrile solutions [3, 4]. In this presentation it will be demonstrated that similar aminomalononitrile based films can be obtained by electropolymerization [5]. The mechanism of the film deposition and their morphology (Figure) will also be described. In particular we will show that films can also be deposited at liquid-air interfaces but having a morphology and a composition different from that deposited at solid-liquid interfaces.



A: water contact angles of AMN based films as a function of the deposition time, and B, C: film morphology after 1 and 19 h as characterized by SEM (B) and AFM (C).

[1] H. Lee, S.M. Dellatore, W.M. Miller, P.B. Messersmith, *Science* **2007**, 318, 426.
[2] S.L. Miller, *Science* **1953**, 117, 528.
[3] H. Thissen, A. Koegler, M. Salwicczek, C.D. Easton, Y. Qu, T. Lithgow, R.E. Evans, *NPG Asia Materials* **2015**, 7, art e225.
[4] D.J. Menzies, A. Ang, H. Thissen, R.A. Evans, *ACS Biomater. Sci. & Eng*. **2017**, 3, 793-806.
[5] V. Ball, RJ. Toh, N.H. Voelcker, H. Thisssen, R.A. Evans, *Colloids & Surf. A.* **2018**, 552, 124.

Invited Speakers

I1. Thermally activated processes and bias field effects on the electrical properties of $BiFeO_3$ thin films

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The effective technological application of bismuth ferrite ($BiFeO_3$) thin films are still limited due to their large leakage current at room temperature. The mechanisms behind the leakage current in $BiFeO_3$ are often associated to the inhomogeneities associated to the Bi volatilization during synthesis, the valence fluctuation of Fe ions and the formation of oxygen vacancies. This work reports the effects of stoichiometry control, secondary phases and oxygen vacancies on the electrical properties of $BiFeO_3$ thin films with different dielectric responses prepared by chemical solution. Thermally activated processes and bias electric field effects on the studied films will be discussed based on the electrical measurements from impedance spectroscopy and electric modulus spectroscopy, carried out in the frequency (100 Hz to 1 MHz) and temperature (300 K to 480 K) range. Results suggest that long-range and localized relaxation coexists in thin films with secondary phases, such that the activation energies of conduction were 0.46 and 0.47 eV for grain and grain boundary, respectively. On the other hand, for monophasic film post annealed in oxygen the activation energy of conduction increases to 0.68 eV. The lower activation energies were attributed to the first ionization of oxygen vacancies while higher to the second ionization of oxygen vacancies. Dielectric dispersion measurements as a function of dc electric field (0 to 20 $kV.cm^{-1}$) within the same frequency range revealed a similar dielectric relaxation like observed as a function of the temperature. The results demonstrated that the control of intrinsic defects during the synthesis strongly impacts the dielectric response and conductivity of $BiFeO_3$ thin films.

I2. Piezoelectric and ferroelectric properties of various amino acids and dipeptides structures: molecular modeling and experiments

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All amino acids have own dipole moments, which interact one another during self-assembling of the amino acids or their dipeptides into more complex molecular structures, such as ion channels [1] in biological membranes, or, for example of dipeptide nanotube (PNT) [2], in material science and medicine. Now many of these structures, exerting the bioferroelectric properties [3] were studied with different methods as experimentally as well theoretically. One of the useful approach is computer molecular modeling, which allow us to calculate and predict main physical properties of these structures. Diphenylalanine (FF) PNTs were considered recently using molecular modeling by quantum-chemical PM3 method (in HyperChem software) and by experimental Atomic force microscopy (AFM)/piezo-response force microscopy (PFM) measurements [3]. But not only FF PNTs, having aromatic rings, can demonstrated ferroelectric properties. As pointed out by Leuchtag [1] the branched-chain amino acids (BCAAs) isoleucine (I), leucine (L) and valine (V), are known to exhibit ferroelectric properties with extremely large values of spontaneous polarization and dielectric permittivity [4]. In present work the piezoelectric and ferroelectric properties of the PNTs on the the BCAAs based dipeptides such as di-isoleucine (II), di-leucine (LL) and combined alanine-isoleucine (AI) dipeptides were studied by similar molecular modeling by PM3 method, as well by experimental AFM/PFM measurements. Now, the only α-helix conformations and L-chiral initial BCAAs molecules were considered in this work now. D-chiral as well β-sheet conformation will be considered later. From experimental X-ray measurements was known that FF PNT have shape of the isolated ring with six dipeptides, which form the parallel stacking of two rings into the crystal hexagonal structure [2] and into two layering rings in tubular models of these PNTs [3]. However, for PNTs with BCAAs only four dipeptides can form the similar isolated ring and construct the crystal structure [2], as well similar tubular models of PNT[3]. After optimization of constructed models by the Polak – Ribiere conjugate gradient method (from HyperChem), the total dipole moment and polarization of PNTs were calculated, with strong orientation along main c-axis of PNTs and values: P_z (*LL*) ~ 3.6 μC/cm^2, P_z (*II*) ~ 6 μC/cm^2, P_z(*AI*) ~ 8.02 μC/cm^2. As it was known for FF PNT the biggest polarization (for L-chiral and conformation β) is P_z ~ 4 μC/cm^2 [3]. These polarizations allow to estimate the piezoelectric coefficients d_{33} along c-axis (in accordance with known electromechanical coupling relationship): d_{33}*(LL)* ~ 44 pm/V, d_{33}*(II)* ~ *73* pm/V, d_{33}*(AI)* ~ *99* pm/V, which are comparable with known data for FF PNT d_{33}*(FF)* ~ *50* pm/V [3]. These data obtained were confirmed by experimental AFM/PFM observations and measurements. Authors wish to acknowledge the Russian Foundation for Basic Researches (RFBR) grant # 19-01-00519 A, and the Portuguese Foundation for Science and Technology (FCT) for the financial support: IF/00582/2015, BI (DOUTOR)/6323/2018).

[1] H.R. Leuchtag, Ferroelectrics, 236, 23-33 (2000)
[2] C.H. Gorbitz, Chem Eur J., 7, 5153–5159 (2001).
[3] V.S. Bystrov, S.A. Kopyl, P. Zelenovskiy, et al, Ferroelectrics, 525, 168–177 (2018)
[4] A. Chen, C-D. Poon, T. Dingemans, et al, Liquid Crystals, 24, 255-262 (1998)

I3. Strong piezoelectricity in Pirydyl-Alanine based hybrid crystals

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New amino acid based [H-β-(X-pyridyl)-Ala-OH][ClO_4], where X=2,3,4 crystals were synthesized and their structure and functional piezoelectric properties were investigated in detail. 2-pyridyl derivative crystallizes in the piezoelectric $P2_12_12_1$ space group whereas the two latter belongs to the polar $P2_1$ space group. Piezoelectric force microscopy (PFM) measurements revealed that the shear piezoelectric coefficient, of the [H-β-(3-pyridyl)-Ala-OH][ClO_4] crystal is more than twice that in the widely used transducer material lithium niobate. The crystal structures of crystals under investigation are characterized by inter- and intramolecular hydrogen bond networks. The existence of intramolecular hydrogen bonding was confirmed by means of IR measurements. The thermogravimetric (TGA) technique was applied to study the thermal behaviour of the title crystals. The piezoelectric properties are discussed in the context of the crystallographic structure and the microstructure of the crystals.

References

[1] M. Wojtaś, A. Gągor and A. L. Kholkin, J. Mater. Chem.C, **4**, 7622 (2016)

[2] M. Wojtaś, V. Kinzhybalo, I. Bdikin, and A. L. Kholkin, Cryst. Growth Des. **19**, 2583 (2019)

I4. Electronic structure calculations of solids, surfaces and nanostructures

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Density functional theory has been a trustful workhorse whenever there is a need to theoretically reproduce a wide range of experimental observables. It gives us access to a quantum-mechanical picture of an electronic gas under the influence of thousands of nuclei. Density functional theory and spectroscopy techniques are, in many aspects, inseparable partners in a modern laboratory, and played decisive roles in the identification and understanding of a vast amount of problems on solid-state physics, surface science and nano-technology. In this talk I will explain the workflow of DFT modeling, why it has been so successful, and along the way, a few successful stories will be told, including how we found the workings of major carrier-life-time-limiting traps in SiC power devices [1,2], the flipping-dynamics of reconstructions on semiconductor surfaces [3], the recent identification of the defect responsible for the light-induced degradation of the power conversion efficiency of Si solar cells [4], or the mechanism for electron-transfer within a network of silicon nanocrystals [5].

References

[1] J. Coutinho, V. J. B. Torres, K. Demmouche, and S. Öberg, *Physical Review B* **96**, 174105 (2017).
[2] I. Capan, T. Brodar, J. Coutinho, T. Ohshima, V. P. Markevich, and A. R. Peaker, *Journal of Applied Physics* **124**, 245701 (2018).
[3] R. Zhachuk, J. Coutinho, K. Palotás, *Journal of Chemical Physics* **149**, 204702 (2018).
[4] M. Vaqueiro-Contreras, V. P. Markevich, J Coutinho, P. Santos, I. F. Crowe, M. P. Halsall, I. Hawkins, S. B. Lastovskii, L. I. Murin, and A. R. Peaker, *Journal of Applied Physics* **125**, 185704 (2019).
[5] R. N. Pereira, J. Coutinho, S. Niesar, T. A. Oliveira, H. Wiggers, M. J. Rayson, P. R. Briddon, M. S. Brandt, M. Stutzmann, *Nano Letters* **14**, 3817 (2014).

I5. Self-standing chitosan-based piezoelectric composite films

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Actuators, sensors and energy generators are key technologies to implement the "Internet of Everything". The motivation of this work is the preparation of a bionanocomposite for biocompatible piezoelectric materials applicable as actuators, sensors or generators. Chitosan, which is a polysaccharide with the ability to form films, is used as matrix and lead-free barium titanate particles, a ferroelectric and piezoelectric material at room temperature, are used as fillers. The $BaTiO_3$ particles are synthesized by hydrothermal method during 24 h at 200 °C. The structural characterization by X-ray diffraction (XRD) and Raman spectroscopy allowed us to verify that the particles synthesized at 200 °C show a well-defined tetragonal crystallographic structure after 24 hours of synthesis. The particles display uniform cubic morphology and average size of about 300 nm. The films are obtained by the solvent evaporation method, after dispersing the particles in different proportions, in the chitosan solution. The addition of particles improves the mechanical properties of the chitosan films, making them more resistant, elastic and ductile. These films were more resistant to water than pure chitosan films, revealing the interaction between the particles and the chitosan matrix. In relation to the electric behavior of the films, the increase of particles improves the permittivity of the samples five times in relation to the biopolymer material. The bionanocomposites developed based on chitosan and barium titanate are promising alternatives to synthetic polymers.

Acknowledgement

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I6. High capacity hydrogen storage: current developments and future perspectives

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Abstract:

It is necessary to identify a most suitable hydrogen storage material for optimizing the fuel tank for H_2 fuel cell vehicles. In this context, we have studied a few important solid state materials and concludes that presently $NaAlH_4$ and MgH_2 (reversible capacity: 5.5 wt.% and 7.4 wt.%) are the two best systems for applications.

Introduction:

As per the DOE target for H_2 vehicles, for achieving a commercial success in the year 2025 the hydrogen fuel tank should be capable of delivering a capacity of 5.5 wt.% H_2 at the temperature of 85 °C (maximum value) and pressures, 5 - 12 bars. Currently, due to thermodynamic restrictions none of the materials investigated so far exclusively satisfy this target. Nonetheless, with few exceptions, the reversible hydrides such as sodium alanate (capacity: 5.5 wt.%) and magnesium hydride (capacity: 7.4 wt.%) seems interesting systems. Among these two, MgH_2 receives much attention because of its higher capacity. MgH_2 releases hydrogen endothermically with a heat change of 74 kJ/mol.H_2 following the reaction $MgH_2 \leftrightarrow Mg+0.5H_2$.[1] The equilibrium temperature (T_{eq}) correspond to the heat change of 74 kJ/mol.H_2 at 1 bar pressure is 282 °C for the above reaction. At this temperature and pressure, due to high activation energy (E_a, 195 kJ/mol.H_2) pristine MgH_2 bulk particles release only a trace amount of hydrogen with very poor kinetics. In order to improve the hydrogen ab/de-sorption kinetics, we employed Nb_2O_5 and TiO_2 additives and observed that the kinetics of MgH_2 can be improved by more than 5 orders of magnitude at ~300 ºC as compared to the additive free sample. Titania especially was also identified to be a promising additive for $NaAlH_4$ system. Presently our future choice is reactive hydride composite system, $LiBH_4 + 0.5MgH_2 \leftrightarrow LiH + 0.5MgB_2 + 2H_2$ offering 11.4 wt.% reversible H_2 capacity.

Experimental:

The rock salt $Mg_xM_yO_{x+y}$ (M=Nb, Ti) was synthesized by the mechanochemical reaction between MgH_2 and Nb_2O_5/TiO_2 using Retch PM200 planetary milling facility. The additive was ball milled with the hydrides under inert atmosphere for 2h at 350 rpm. Hydrogen storage measurements were performed by using Sieverts volumetric facility. The samples were characterized by XRD, XPS, AFM and SEM facilities available in our laboratory.

Results and Discussion:

MgH_2 was catalyzed by a 3 wt.% of Nb_2O_5 and TiO_2 by mechanochemical treatment for 2h.[2] Our detailed studies prove that both these oxides actually interacts with MgH_2 and makes a catalytically activity in-situ product with a typical formula of $Mg_xM_yO_{x+y}$ (M=Nb, Ti). The in-situ additive $Mg_xM_yO_{x+y}$ play as a catalyst and improves the de/re-hydrogenation kinetics of MgH_2 by at least 5 orders of magnitude. Detailed studies also suggest that if the size of MgH_2 particles is reduced down to a few tens nanometer (typically <50 nm) better performance can be achieved and no additive is necessary. However, due to the high tendency of agglomeration of MgH_2 particles, it becomes bulk again in few cycles and apparently the system releases H_2 with poor kinetics. Studies performed by our team and worldwide researchers proves that impregnating MgH_2 on the pores of scaffold materials is the best strategy for addressing this issue.

Regarding $NaAlH_4$, the kinetics of this system is a crucial issue but that can be improved by incorporating suitable additives. We tested the effect of loading oxide additives (2 mol.%) such as TiO_2, CeO_2, La_2O_3, Pr_2O_3, Nd_2O_3, Sm_2O_3, Eu_2O_3 and Gd_2O_3 with $NaAlH_4$ and observed that TiO_2 is the best additive. It was also found that when the size of TiO_2 additive nanoparticles was reduced from 200 nm to 5 nm, not only the kinetics of hydrogen release from $NaAlH_4$ can be improved but also the stable intermediate phase Na_3AlH_6 can be destabilized at temperatures as low as 150 ºC.

Our present studies are aimed at improving the hydrogen storage performance of another promising RHC system $LiBH_4$ + $0.5MgH_2$ through nanoconfinement strategy.

Conclusion:

Presently, none of the high capacity solid state metal hydrides satisfy all the target conditions for H_2 FC vehicles. However, a few metal hydrides, as for example MgH_2, can be deployed for H_2 tanks by incorporating an external heating device. Using MgH_2 one can obtain a reversible capacity of 6 – 6.5 wt.% H_2 at 300 °C temperature and <10 bar pressure but it can only be a short term option. In order to reach the "ultimate target" (long term target), it is necessary to develop hydrogen storage materials capable of consistently restoring >10 wt.% H_2. Few irreversible materials with 10 – 20 wt.% H_2 capacity are known in the literature but these materials require elaborate further study. We believe that two directions show considerable promise for future developments, (i) tailoring new high capacity RHCs and improving the existing RHC systems, (ii) modification of reaction route for obtaining direct reversibility for high capacity irreversible hydrides (e.g., NH_3BH_3, $LiAlH_4$, AlH_3, $Mg(AlH_4)_2$, $LiBH_4$ etc). Any breakthroughs in directions (i) and/or (ii) will make hydrogen economy a practical reality.

Acknowledgement

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References

1. D. Pukazhselvan et. al, Nano Energy 1, 566 (2012)
2. D. Pukazhselvan et. al, Appl. Surf. Sci. 420, 740 (2017).

I7. Dynamic of molecules rotation in monolayer C_{60} film

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The motion of single atoms or molecules plays an important role in nanoscale engineering at the single atomic or molecular scale. Effect of molecule center mass displacement on conductivity of C_{60} based junction has been previously reported [1]. Understanding of molecular motion is crucial to further progress in molecule-based nano-electronic devices. The symmetry and deviations from a spherical shape of the C_{60} molecule generate the rotational degrees of freedom which often determine physical and structural properties of compounds, C_{60} based clusters and crystal.

We employed STM to reveal switching of individual C_{60} between different orientations within a single molecular layer grown on the WO_2/W(110) surface (Fig. 1a-e). Switching of the molecule between orientations resulted in a telegraph noise in tunneling current (Fig. 1d) or in Z position of STM probe. Statistics of switching has been used to determine energy gap and potential barrier height between two adjacent orientations of the molecule.

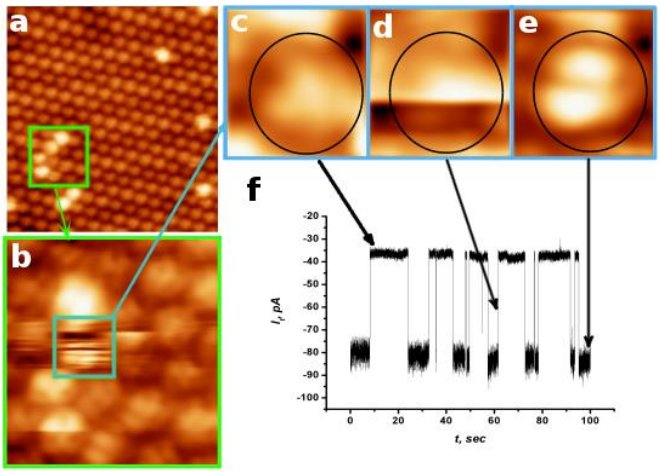

Fig. 1. STM images of the C_{60} monolayer, Vb= 1.25 V, I= 3 nA, and T= 85 K. (a), (b) Change in the state of a single C_{60} molecule; (c), (e) images of two different orientations of a molecule; (d) image of a molecule during its switching between two orientations; and (f) time evolution of tunneling current

Rotational transitions in single molecular layer of C_{60} were also studied. Rotational first order phase transition at T_C=260K has been established [2]. Above that temperature molecules continuously rotate around their centres of mass whereas below T_C the rotational degree of freedom is suppressed and C_{60} molecules undergo thermally activated switches between closely positioned in energy orientations. The rate of jumps rapidly decreases with decreasing temperature and at 220 K the molecules stay in each state for longer than the time of a possible experiment. Therefore, a kinetic glassy transition can be identified at 220 K. The integrity of the monolayer of C60 molecules is not altered once the molecules transition to the spinning state, but remarkably, the separation between the molecules and surface is increased by 1.2 Å across the transition. The energy of the spinning state with respect to the lowest energy state having coordinated bond can be obtained from statistics of the molecule's switching. The binding energy of the molecule in the spinning state can be easily altered by changing the polarity of the bias voltage applied between the STM tip and the surface. The binding energy is decreased by 80 meV when the bias polarity of the sample changes from positive to negative with respect to the tip. The results are consistent with the Coulomb blockade model: when electrons travel from the surface to the C60 molecule and then to the tip, they produce an accumulation of charge on the molecule due to the Coulomb blockade. This increases the electrostatic interaction between the molecule's charge and a corresponding image charge created on the metallic surface. The energy of this electrostatic interaction is consistent with the energy difference of the spinning state for positive and negative bias voltage polarity.

[1] Hongkun Park, et.al., Nanomechanical oscillationsin a single-C60 transistor, Nature, 407, 57, 2000; N.Neel, et.al. Two-level conductance fluctuations of a single-molecule junction, Nano letters, 2011, 11, 3593

[2] Sergey I. Bozhko et.al. Rotational transitions in a C_{60} monolayer on the WO_2/W(110) surface, Phys. Rev. B. 84,195412, (2011)

I8. Strain mediated substrate effect on the properties of polar dielectric thin films

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Low cost scalable processing and substrates are critical for optimized polar dielectric performance of functional oxide thin films if they are to achieve commercialization. Here, a comprehensive investigation of the role low-cost MgO, Al_2O_3, $SrTiO_3$ and Si substrates on the structural and electrical properties of sol-gel derived $SrTiO_3$ (ST) and $K_{0.5}Na_{0.5}NbO_3$ (KNN) thin films is presented. The substrate is found to have a strong effect on the stress/stain state and, consequently, on the dielectric and ferroelectric response of the films. A tensile stress induced in-plane by the thermal expansion mismatch between the substrates and the films observed for ST and KNN films deposited on platinized Al_2O_3 and Si substrates, respectively, lowers the relative permittivity and remanent polarization values in the parallel plate capacitor geometry. In contrast, a compressive stress/strain observed for ST films deposited on MgO/Pt and KNN films on $SrTiO_3$/Pt substrates result in superior polarization and dielectric permittivity, corresponding to enhanced out-of-plane displacement of Ti^{4+} ions in ST films and Nb^{5+} ions in KNN films. It is thus demonstrated that for polycrystalline polar dielectric thin films the relative permittivity and polarization may be optimized through an induced compressive stress state [1,2].

References

[1] A. Tkach, O. Okhay, I.M. Reaney, and P.M. Vilarinho, *J. Mater. Chem. C*, **6**, 2467 (2018).
[2] A. Tkach, A. Santos, S. Zlotnik, R. Serrazina, O. Okhay, I. Bdikin, M.E. Costa, and P.M. Vilarinho, *Coatings*, **8**, 449 (2018).

I9. Utilizing reduced graphene oxide for harvesting / storage energy

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The need for clean and sustainable energy sources to meet the exponentially rising energy demands of the world has compelled scientists to look for new power generation strategies. Solar cell and thermoelectric (TE) energy conversion have the advantage to harvest widely distributed waste heat and are also proved as an alternative route to convert solar/thermal energy into electric power economically [1]. At the same time the renewal of interest to fundamental mechanisms of energy storage in electrochemical supercapacitors (SCs) was boosted by the progress in development of novel materials for nanostructured electrodes [2]. SCs can be charged faster than batteries, leading to a very high power density, and do not lose their storage capabilities over time. The main shortcoming of SCs is their low energy density. Preliminary design criteria and cell specifications are following: flexible, low weight and cheap. Reduced graphene oxide (rGO) has attracted significant attention in recent years due to its extraordinary physical and chemical properties [2]. In the current work structural properties, electric, thermoelectric, electrochemical characteristics of rGO-based films and papers are studied and presented.

References

[1]. M.H. Elsheikh, D.A. Shnawah, M.F.M. Sabri, S.B.M. Said, M.H. Hassan, M.B.A. Bashir, and M. Mohamad, *Renewable and Sustainable Energy Reviews*, **30**, 337 (2014)
[2]. Z. Lei, I. Zhang, N.A. Kumar, and X.S. Zhao, *Energy Environ Sci*, 9, 1891 (2016)

I10. Oxide thermoelectrics: redox tuning of the functional properties

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Since most of the energy (~60-70 %) used in the world is discharged as waste heat, the "green" thermoelectric conversion has received a considerable attention due to its intrinsic simplicity, employing no moving parts, silent operation and excellent scalability and reliability. Driven by a need to develop low-cost and thermally stable materials for thermoelectric applications, oxides are considered as a promising alternative to traditional thermoelectrics. Compared to those, oxide materials possess a unique redox flexibility and defect chemistry, which can be precisely set-up by controlled heat treatment combined with oxygen partial pressure changes. This work demonstrates how, by redox-sensitive substitutions, the thermoelectric properties of oxides can be tuned and enhanced. The developed strategies are exemplified by considering tungsten- and molybdenum- co-substituted strontium titanate, prepared under strongly-reducing conditions. In-situ formation of nanocomposite and atomic-scale inhomogeneities composed of $SrMoO_3$-based insertions into $SrTiO_3$ perovskite lattice promote simultaneous significant increase in the power factor and decrease in the thermal conductivity by decoupling the thermal and electrical properties. The proposed approaches show good prospects for tailoring thermoelectric performance in other oxide-based systems, containing redox-active cations.

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I11. Magnetization reversal and low temperature magnetocaloric effect in rare-earth orthochromites: Impact of doping

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Rare-earth orthochromites have gained significant attention worldwide during this decade because of their rich physics and potential applications in spintronics, thermomagnetic switches, photocatalyst, solid-state fuel cells [1-3]. $SmCrO_3$ (SCO) belonging to this exotic class of materials has shown to be a multiferroic compound with peculiar magnetic properties along with ferroelectric nature. The appearance of magnetization reversal in this compound is still under debate. This material also demonstrates exchange bias, spin reorientation transition, positive and negative magnetocaloric effect at low temperatures [1]. However, the observed magnetocaloric effect, in the pristine compound, is quite small hindering its application as a low temperature solid-state magnetic refrigerant [1]. In this talk, we shall focus about the possible ways of inducing magnetization reversal and enhancing the magnetocaloric effect through proper chemical substitution in rare-earth orthochromites such as $SmCrO_3$. The effect of doping of different ions on the structural, electrical, optical and magnetic properties will also be discussed.

References

1. P. Gupta and P. Poddar, Study of magnetic and thermal properties of $SmCrO_3$ polycrystallites, RSC Adv. 6 (2016) 82014–23.
2. S. Kumar, I. Coondoo, M Vasundhara, A. K. Patra, A. L. Kholkin and N. Panwar, Magnetization reversal behavior and magnetocaloric effect in $SmCr_{0.85}Mn_{0.15}O_3$ chromites, J. Appl. Phys.121 (2017) 43907.
3. N. Panwar, I. Coondoo, S. Kumar, S. Kumar, M. Vasundhara and A. Rao, Structural, electrical, optical and magnetic properties of $SmCrO_3$ chromites: Influence of Gd and Mn co-doping, J. Alloys Compd. 792 (2019) 1122.

I12. An investigation on the impact of the synthesis routes on the electrical properties of lead-free ceramics

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The influence of synthesis methods on the electric properties of lead-free piezoelectric ceramics $(Ba_{0.85}Ca_{0.15})(Zr_{0.10}Ti_{0.90})O_3$ (BCZT) fabricated via chemical and conventional oxide methods has been systematically investigated [1]. It was observed that the average grain size estimated from the microstructure was ~1.5 µm in the sol-gel derived ceramic (SG BCZT) which was much smaller than that obtained in coarse grained (~27 µm) sample prepared by solid-state method (SS-BCZT). Further, grain size was found to have profound impact on various electrical properties viz. dielectric, ferroelectric, piezoelectric and impedance. The increase in grain boundary density enhanced diffuseness while suppressed the dielectric peak in SG-BCZT. Likewise, increase in elastic stiffness and progressive hindrance to domain wall movements, resulted in a decrease of the remnant polarization and the associated piezoelectric charge coefficient values in SG-BCZT sample. Accordingly, higher Young's modulus value of 158.3 GPa was observed in SG-BCZT as compared to 117.9 GPa in SS-BCZT. Local-area piezoresponse force microscopy (PFM) images revealed lamellar domains in SS-BCZT while small sized fractal-like irregular domains were recorded in SG-BCZT. Complex impedance spectroscopy results along with grain boundary conductivity were also understood in terms of grain size effect. The mechanisms of grain size driven effects and their impact on the functional properties of lead-free piezoelectrics will be discussed.

References

1. I. Coondoo, N. Panwar, D. Alikin, I. Bdikin, S.S. Islam, A. Turygin, V.Y. Shur, A.L. Kholkin, A comparative study of structural and electrical properties in lead-free BCZT ceramics: influence of the synthesis method, Acta Materialia 155 (2018) 331-342.

I13. Hollow BN spherical nanoparticles: synthesis and applications

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Nanoparticles of spherical morphology find many areas of application now, significant usages are at the moment are actively developing in biological, medical and ecological fields. Due to excellent physical-chemical properties of boron nitride, applications of its nanospheres can significantly expand areas of utilization. The question of present interest in regards of such nanoparticles is the development of high yield synthetic method which may produce particles of homogenous size. In the present work the new nanomaterial consisting of hollow spherical BN nanostructures with smooth and petal-like surfaces was obtained for possible applications in composite materials and as drug delivery containers.

Synthesis of BN nanospheres with an external diameter of 80-250 nm was carried out by CVD method using boron oxide vapor and flowing ammonia in a BN ceramic reactor placed in a vertical induction furnace. Three types chemical compound powders with a different ratio of constituents were used as a source of B_2O_2 vapor. The temperature in a location area of the precursor was varied over the range of 1200-1430°C. Synthesis was carried out for 200-420 min. Products of syntheses were collected on the walls of BN crucible in a low temperature zone out of BN reactor as a thick light snow-white material. Typically, using 10 g of the precursor was enough to synthesize about 250-400 mg of the material in 420 min.

As was revealed by SEM analysis, the synthesized powders obtained in all experimental conditions consist of agglomerates of spherical nanoparticles with a hollow core and an average size 80-200 nm, and a petal-like surface made of nanosheet-like flakes. After some syntheses hollow spherical particles with smooth surface were also observed. The synthesized products were proved to be of the BN phase with a hexagonal structure using EDX, XRD and FTIR methods. It was shown that the experimental conditions mostly affected the impurity content and the yield of the nanomaterial product. TEM analysis shows that nanoparticles exhibit a hollow spherical central part and a petal-like surface due to exposed BN layers at the side area.

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I14. The Relation between the Material Mechanical Properties and the Behaviour in the Fluid-Solid Structures Interaction

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The more complicated Fluid-structure interaction (FSI) form is cavitation collapses on/near the structure. In this lecture, the investigation and analysis of ductile materials behavior under FSI process and cavitation bubble collapsing mechanisms will be presented and discussed. Three ductile materials (Cu, AlMnMg-alloy, and St.St.316) were treated with cavitation under the same working conditions but for different exposure time. The influence of fluid temperature was also tested. The cavitating jet generator as a tool experience intensive, fast and vary intensity levels cavitation phenomenon which is suitable for FSI process study. A commercial-purity copper was used as tested material to investigate the effects of the hydrodynamic and geometrical parameters on the FSI process, their influence on the cavitation characteristics is also discussed based on the evaluation of the FSI result. The treated materials were submitted to different microscopy techniques and surface morphology analysis was done. The obtained result shows that the damage process is created by the shearing stress on the surface induced by the microjets which are created as a result of cavity collapse on or near the surface. The mechanical properties of the material mainly “fatigue strength” and its stacking fault energy played a major role in the damage process. The damage levels based on exposure time period are presented. The microscopy techniques provide significant information for monitoring and understanding the damage mechanism and progress. Energy-dispersive X-ray spectroscopy (EDS) helps in the interpretation of the material's behavior. Also, it was found that the tested parameters have a strong influence on the FSI rate, FSI area, Strength FSI damage, and the kind of damage. A comparison between the obtained results explains some of the mechanisms involved in cavitation, FSI process, damage and their relation to the tested parameters. Mathematical expressions which combine these parameters with the damage rate are obtained. These parameters are very important in order to control the FSI, cavitation as a phenomenon and also to improve the performance of the cavitating jet generator. a model of the FSI and damage process stages is proposed describes different stages.

References

[1] Hutli E., et al. Archive of Applied Mechanics, Vol. 78, pp.329-341,2008
[2] Hutli E. et al. Plasmonics –international journal for Nano Sciences springer, Vol. 8. pp. 843-849,2013
[3] Hutli E. et al., THERMAL SCIENCE: Scientific journal, Vol. 17, pp 1151 – 1161,2013
[4] Hutli E. et al., THERMAL SCIENCE: Scientific journal, Vol. 17, pp. 1139-1149, 2013
[5] Hutli E. et al., Tribology International, ELSEVIER, Vol. 101, pp. 88–97,2016
[6] Hutli E. et al., Mechanics of Materials, ELSEVIER, Vol. 92, pp. 289–298,2016
[7] Hutli E. et al., International Journal of Multiphase Flow, ELSEVIER,Vol. 83, pp.27–38, 2016
[8] Hutli E. et al., Experimental Thermal and Fluid Science ELSEVIER, Vol. 80, pp. 281–292, 2016
[9] Hutli E. et. al., International Journal of Heat and Mass Transfer, ELSEVIER Vol.117, Pp. 873-886, 2017
[10] Hutli E. et al., Applied Surface Science, ELSEVIER, Vol. 458, pp. 293-304, 2018

I15. Chirality-dependent self-assembly of diphenylalanine microtubes

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Chemical and physical aspects of chirality are of ongoing research interest. The chiral-induced spin selectivity effect was used recently to manipulate electron spins transmitting through short organic molecules [1] and long supramolecular structures [2,3]. Practical applications of chirality-dependent properties require their detailed study in various chiral supramolecular systems. Peptides are convenient building blocks for creation of various supramolecular structures via self-assembling: from vesicles and nanospheres to nanotubes, nanobelts and thin films. Such structures possess chirality at different hierarchical levels of organization and are considered as advanced functional materials for nanotechnological and biomedical applications. The simplest and most studied self-assembled dipeptide is diphenylalanine (H-Phe-Phe-OH, FF), which easily forms nanotubes and microtubes demonstrating high rigidity [4,5], piezoelectric [6] and pyroelectric properties [7].

Here we demonstrated the difference in crystal structure and growth kinetics of FF microtubes formed from L- and D- enantiomers investigated experimentally and theoretically by computer simulation. The microtubes of L- and D- enantiomers were grown simultaneously and under identical experimental conditions, however they possess different crystallographic space groups, have essential difference in sizes and demonstrate different growth kinetics. Computer simulation by means of molecular mechanics methods revealed fundamental difference in interaction between structural units of microtubes of different chiralities.

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References

[1] R. Naaman, D.H. Waldeck, *Annu. Rev. Phys. Chem.*, **66**, 263 (2015).
[2] M. Kettner, B. Göhler et al., *J. Phys. Chem. C*, **119**, 14542 (2015).
[3] B. Göhler, V. Hamelbeck, T.Z. Markus et al., *Science*, **331**, 894 (2011).
[4] N. Kol, L. Adler-Abramovich, D. Barlam et al., *Nano Lett.*, **5**, 1343 (2005).
[5] P. Zelenovskiy, I. Kornev et al., *Phys. Chem. Chem. Phys.*, **18**, 29681 (2016).
[6] A. Kholkin, N. Amdursky et al., *ACS Nano*, **4**, 610 (2010).
[7] A. Esin, I. Baturin, T. Nikitin et al., *Appl. Phys. Lett.*, **109**, 142902 (2016).

I16. Crystal structure of co-doped $BiFeO_3$ ceramics near the phase boundary regions

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Multiferroics based on bismuth ferrite attract much attention of the scientific community due to the high temperature of ferroelectric-paraelectric transition and substantial temperature stability of magnetically active state [1-4]. The diverse phase transitions observed for the $BiFeO_3$-based compounds are reflected in numerous phase diagrams which assume a strong coupling between the crystal structure and physical properties of the materials.

An example of system $Bi_{1-x}Ba_xFe_{1-x}Ti_xO_3$ it is shown nontrivial evolution of the crystal structure of the $BiFeO_3$-based compounds near the morphotropic phase boundary regions.

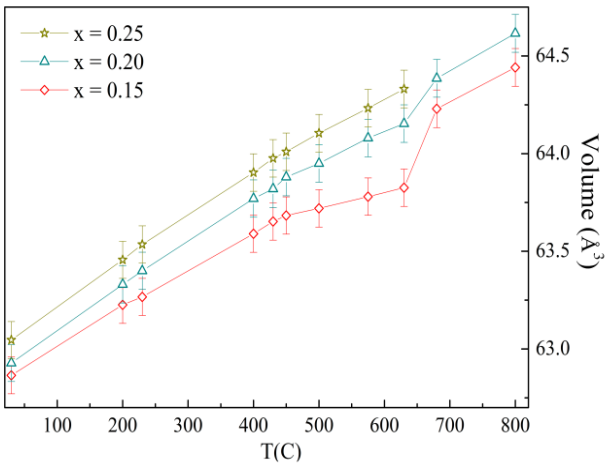

Fig.1. Temperature evolution of the averaged primitive cell volume estimated for the compounds $Bi_{1-x}Ba_xFe_{1-x}Ti_xO_3$.

It has been found that increase in the dopant concentration gives rise to the reduction in rhombohedral distortion of the unit cell, causes its expansion, and leads to the formation of single phase pseudo-cubic state via the two-phase region attributed to the concentration range $0.2 \le x \le 0.25$. Temperature increase (Fig. #1) results in the stabilization of the single phase cubic state in the compounds having the dominant pseudo-cubic structure at room temperature. The compounds having the dominant rhombohedral structure at room temperature ($x \le 0.15$) demonstrate an unexpected strengthening of the rhombohedral distortions at elevated temperatures; a further temperature increase causes the phase transformation into the single phase cubic structure.

References

[1] S. M. Selbach et al., J. Solid State Chem. **183**, 1205 (2010).
[2] D. V. Karpinsky, et al., npj Comput. Mater. **3**, 20 (2017).
[3] G. Catalan and J. F. Scott, Adv. Mater. **21**, 2463 (2009)
[4] D. V. Karpinsky et al., J. Am. Ceram. Soc. **97**, 2631 (2014)

Oral presentations

O1. Mechanical properties of polypropylene bio composites with sea weeds

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The interest in the utilization of bio-fillers in thermoplastics has increased recently, mainly due to the need in overcoming the environmental problems caused by the agricultural by products. Based on former exploratory research, we used seaweed fiber as a novel biofiller for the production of polypropylene (PP) biocomposites. Maleic anhydride grafted PP was applied as compatibilizers. The incorporation of the bio fillers at compositions ranging from 10-30% was carried out by melt compounding in extruder and then injection molded into standard test samples. Mechanical and physical characteristics of the composite systems were studied to evaluate the effect of seaweeds content on PP. It has been found that while there is a decrease in elasticity modulus, tensile strength at break and elongation ect, the hardness and melt flow index were found to be increased with the seaweed content.

References

[1] E. Bodors, C. Baley, Mater Lett 62, p.2143,(2008).
[2] M. A. Mydul, A. Toufiq, H. Monimul, Polym Plast Technol Eng 42, p.110, (2009)
[3] G. Sui, M. A. Fuqua, C.A. Ulven, W. H. Zhong, Bioresource Technol 100, p.1246 (2009)
[4] S. V Joshi, L. T. Drzal, A. K Mohanty, S. Arora, Compos Part A 35-3, p.371. (2004)
[5] G. Alexandre, M. Takanori, G. Koichi, O. Junji, Compos Part A 38, p. 1811. (2007)
[6] N. Hatta, N. Akmar, CUTSE International Conference 24-27 November (2008) Malaysia.
[7] B.S. Ndazi, C. Nyahumwa, Tesha , J. Bio Resources 3(4), p. 1267, (2007)
[8] A.S.Murtuza, International Conference on Advances in Polymer Technology, Feb 26-27, (2010) India, pp.60
[9] M. Shahril Ezuan Mustapa, Azman Hassan and Abdul Razak Rahmat, Simposium Polimer Kebangsaan Ke-V. Ogos 23-24, (2005)
[10] P. A. Sreekumar, P. Albert, G. Unnikrishnan, K. Josepy, S. Thomas, J Appl Polym Sci 109, p. 1547, (2008)
[11] A. M. S. Silva, K. G. K. Fermoseli, M.A.D. Paoli, J Appl Polym Sci 112, p. 3686, (2009)
[12] A. S. Shigha, KV.K. Thakur, Polym Plast Technol Eng 48, p.201 (2009)

O2. Piezoelectric, ferroelectric, optoelectronic phenomena in hydroxyapatite by first-principles and influencing of them by the defects levels

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Hydroxyapatite (HAp) is an important component of mammal bones and teeth, being widely used in prosthetic implants [1]. However, despite the importance of HAp in medicine (exciting applications involving this material as a high biocompatible materials [1]), several promising new applications involving this material (e.g., in photo-catalysis [2]), depend on how well we understand its fundamental properties. Recent experiments and theoretical studies have shown that HA exhibits piezoelectricity, pyroelectricity, and ferroelectricity [3-8]. A number of theoretical studies of the structure and properties of HA have been carried out [3-6]. It shown the value of the d_{33} piezoelectric coefficient as 15.7 $pC \cdot N^{-1}$ in good agreement with the experimental study as described in [7, 8]. Further, experimental evidence suggests that oxygen vacancies play a critical role in the production of surface radicals upon exposure of HAp to ultraviolet (UV) light. However, very little is known about the underlying physical and chemical details.

A hybrid density functional theory (DFT) study of the structural and electronic properties of oxygen vacancies in large HAp supercells within the plane-wave formalism was presented in this work.The vacancies were investigated in large supercells, from which formation energies and electronic transition energies were calculated. The calculations were carried out using DFT, as implemented by the VASP [9]. The exchange-correlation potential was evaluated either using the generalized gradient approximation according to PBE functional or the three-parameter hybrid B3LYP functional, which incorporates a fraction of exact exchange with local and semi-local functional [10]. These methods are also applied to the calculation of defect levels [11].

We found that the vacancies essentially occur in two distinct forms, either as a simple vacant oxygen site (referred to as structures I-IV), or as an oxygen atom replacing two neighbouring oxygen vacancies (bridge structures A-C). The former type of vacancies are
deep donors, while the latter are shallow donors with rather low ionization energies. No acceptor states (stable negatively charged defects) were found. Vacancy structures I-IV are more stable in the neutral charge state, while bridge structures A-C are preferred in the double plus charge state. This means that the oxygen vacancy adopts rather different configurations on samples where the Fermi energy is in the upper or the lower half of the band gap. From inspection of the one-electron Kohn-Sham levels, combined with the transition levels obtained from total energies, we find that electron promotion from the valence band top to the donor state of the positively charged structures, involves a zero-phonon absorption of 3.6-3.9 eV.

This transition leads to a spontaneous breaking of either a P-O bridge-bond or an O-H bond, and most likely explains the 3.4-4.0 eV absorption onset for the observation of photocatalysis under persistent UV illumination.

The use of B3LIP allows to consider both electronic excited states of electrons and optical properties, as well as the energy of formation of defects at a high and precise level.

This is not unexpected, since this functionality was developed earlier for the description of molecules, and the studied material based on the hexagonal HAP crystal lattice has a similar molecular structure: it contains isolated PO4 tetrahedra, columns of calcium atoms and OH hydroxyl channel.

The resulting electronic structure of the band of the top of the valence band turns out to be rather flat, which also confirms the "molecular-like" nature of the internal structure of the HAP.
The effectiveness of the use of the exchange-correlation functional B3LYP in the calculations for pure HAP and defect levels in HAP are shown. Further development and more accurate calculation of these electronic properties and optical photoexciting and photocatalytic processes can be made by correct calculations of the electron – electron correlation of the excited electron states taking into account the Frank – Condon relaxation. These contributions are estimated and their results are discussed.The authors thank the Russian Foundation for Basic Researches (RFBR grant 19-01-00519 A) and to the Fundação para a Ciência e a Tecnologia (FCT) through project UID/CTM/50025/2013.

1. Bioceramics and Biocomposites: From Research to Clinical Practice. Ed. A. Iulian. (John Wiley & Sons, Inc., Hoboken, New Jersey), 149-190 (2019).
2. V.S. Bystrov, C. Piccirillo, D.M. Tobaldi, P.M.L. Castro, J. Coutinho., S.Kopyl and R.C. Pullar, *Applied Catalysis B: Environmental* 196, 100–107 (2016).
3. V.S. Bystrov, J. Coutinho, A.V. Bystrova, Yu.D. Dekhtyar, R.C. Pullar, A. Poronin, E. Palcevskis, A. Dindune, B. Alkan, C. Durucan, E.V. Paramonova, *J. Phys. D: Appl. Phys.* 48, 195302 (2015).
4. A. Slepko, A.A. Demkov, AA. Phys Rev B: Condens Matter. 84, 134108 (2011).
5. V.S. Bystrov, *Ferroelectrics* 475 (1), 148-153 (2015).
6. V.S. Bystrov, F*erroelectrics* (7 pages). - (2019) https://doi.org/10.1080/00150193.2019.1574638
7. S.B. Lang et al., Sci. Rep. 3, 2215 (2013).
8. S.B. Lang, *Phase Transitions* 89 (7-8), 678-694 (2016).
9. Vienna Ab Initio Simulation Package (VASP) https://www.vasp.at/ - (accessed 22.11.16 - 23.04.2019)
10. L.A. Avakyan, E.V. Paramonova, José Coutinho, Sven Öberg, V.S. Bystrov and L.A. Bugaev., *J. Chem. Phys.* 148, 154706 (12 pages), (2018).
11. V.S. Bystrov, L.A. Avakyan, E.V. Paramonova, and José Coutinho, *J. Chem. Phys. C.*123 (8), 4856–4865 (2019).

O3. Multi(alkenyl)functionalized silsesquioxanes as potential polysiloxanes modifiers

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Organosilicon compounds are of great interest and have been investigated for almost seven decades which is reflected in the growing numbers of papers and patents published each year. These systems, due to their hybrid i.e. inorganic-organic nature offer development of advanced, multifunctional materials. One of the most popular and worldwide known organosilicon derivatives are Silsesquioxanes, among which the most important are the cubic-type, i.e. T_8 derivatives and recently new- double-decker silsesquioxanes (DDSQ).[1,2]

The aim of this work was to develop efficient and selective methods for the synthesis of mono- and tri(alkenyl)functional cubic-type silsesquioxanes and also di- and tetra(alkenyl)functional double-decker silsesquioxanes basing on hydrolytic condensation and hydrosilylation reactions. These compounds may be exploited as precursors or components for synthesis of new polymeric networks possessing specific features e.g. improved thermal and mechanical properties in comparison to their organic analogues.

References

[1] D. B. Cordes, P.D. Lickiss, F. Rataboul, *Chem. Rev.*, **110**, 2081-2173 (2010).
[2] B. Dudziec, B. Marciniec, *Curr. Org. Chem.*, **21**, 2794 – 2813 (2017).

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O4. SYNTHESIS OF SILICON CARBIDE FILMS BY MAGNETRON SPUTTERING

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In recent years, considerable progress has been achieved in the synthesis of thin epitaxial SiC films on Si by the atomic substitution method [1, 2]. The magnetron sputtering is widespread due to the relatively high growth rates, good adhesion of SiC films and a rather low cost of the technological process [3]. This paper is devoted to the synthesis of solid thick silicon carbide (SiC_x) films on the surface of single-crystal silicon (c-Si) with a thin interlayer of amorphous silicon (a-Si) for better adhesion and to establish new regularities in the influence of heat treatment on composition, crystallization processes and structure of layers. The principal difference in the used synthesis technique from the traditional method of magnetron sputtering is in the high-frequency mode (13.56 MHz) of magnetron sputtering of two targets simultaneously – a silicon target and a graphite target. Using X-ray reflectometry and infrared spectroscopy, it was shown that during the used deposition mode (rf - 150 W, 13.56 MHz; Ar - 2.4 l/h, 0.4 Pa; 100°C, 10800 s) an amorphous SiC_x film of a high density (~ 3.52 g/cm^3) was obtained, significantly exceeding the density of silicon carbide (3.21 g/cm^3). This film contain nanoclusters with a predominance of shortened Si–C-bonds absorbing at 860 cm^{-1}. Using high sensitive photographic X-ray diffraction and infrared spectroscopy, it was shown that rapid annealing (970°C, 5 min, vacuum) leads to a partial decomposition of optically inactive clusters and the formation of Si–C-bonds of tetrahedral orientation which is characteristic of crystalline silicon carbide, and also promotes an improvement of the film structure, formation of α-SiC, β-SiC and Si nanocrystals and reduce the density of the film. Basing on the data of X-ray diffraction and X-ray reflectometry about the phase composition and density of the film (3,522 and 3,397 g/cm^3 before and after annealing), the presence of diamond inclusions and dense clusters in the film was supposed. The unconventional predominance of dense clusters with shortened Si-C-bonds, absorbing at 860 cm^{-1}, is explained by the effect of a high-frequency field, contributing to the formation of small carbon- and carbon-silicon nanoparticles of high density during the film deposition. In the process of rapid annealing, a partial decomposition of these nanoparticles, as well as their low-temperature transformation into α-SiC and β-SiC nanocrystals resulting in a decrease in density and the appearance of X-ray lines of silicon carbide, are taken place.

References

[1] Kukushkin S.A., Osipov A.V., Feoktistov N.A. Synthesis of epitaxial silicon carbide films through the substitution of atoms in the silicon crystal lattice: a review. Phys. Solid State. 56 (8). 2014. P. 1507–1535.

[2] Kukushkin S.A., Nussupov K.Kh., Osipov A.V., Beisenkhanov N.B., Bakranova D.I. Structural properties and parameters of epitaxial silicon carbide films, grown by atomic substitution on the high-resistance (111) oriented silicon. Superlattices and Microstructures. 111. 2017. P.899-911.

[3] Joung Y.-H., Kang H.I., Kim J.H., Lee H.-S., Lee J., Choi W.S. SiC formation for a solar cell passivation layer using an RF magnetron co-sputtering system. Nanoscale Res. Lett. 2012. 7(1):22.

O5. DLC coatings for better orthodontics alloys performance

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Biometals stand out in orthodontics due to the excellent combination of mechanical-chemical-physical properties. However, intraoral environment is extremely aggressive from a corrosion point of view, and inevitably leads to metallic ions release. Free heavy metal ions, such as Ni, Cr, V and Co, can have harmful effects on human health and wellness. [1] In fact, the cytotoxicity of Ni and Cr has been highlighted, and both metallic Ni and its compounds are considered to be carcinogenic according to the International Agency for Research on Cancer, IARC. [2] Also, subtle to severe symptoms of Ni allergic reactions to metallic orthodontic components are described in the literature. [3, 4] It is therefore imperative to develop and implement new strategies in order to minimize those effects without losing biocompatibility of the metallic alloys.
The present work is devoted to Diamond-Like Carbon (DLC) coatings, by magnetron sputtering, as a functional barrier to metal release from biomedical metallic alloys.
The corrosion resistance of DLC films with Cr interlayer for adhesion improvement was studied. The static immersion tests were performed in modified Fusayama-Meyer artificial saliva solution [5] by selecting two pH values (6.8 and 2.3) for 7 or 30 days. Chemical and morphological characterization of the samples were performed by SEM/EDS and AFM, and static contact angles were also measured. The quantification of metallic ions released into the immersion solution baths was obtained by ICP-AES.
The results were very satisfactory, showing that pitting corrosion, which was detected on austenitic stainless-steel substrates, could be avoided by using a DLC-based coating, especially in highly acidic environment. No detachments or relevant morphological/chemical changes of the coating were detected.

References

[1] D. Upadhyay *et al.*, "Corrosion of alloys used in dentistry: A review," *Materials Science and Engineering A*, 432 (1–2), 1–11, 2006.
[2] International Agency for Research on Cancer, IARC, "Nickel and nickel compounds," *IARC Monogr. Eval. Carcinog. Risks to Humans*, 100 C, 169–218, 2011.
[3] O. Kolokitha and E. Chatzistavrou, "A severe reaction to Ni-containing orthodontic appliances," *Angle Orthod.*, 79 (1), 186–192, 2009.

O6. Magnetic iron substitutions in hydroxyapatite: density functional study

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Hydroxyapatite (HAp), $Ca_{10}(PO_4)_6(OH)_2$, is a bio-ceramic material with a calcium-to-phosphorus ratio similar to that of natural bone and teeth. The apatite structure allows the formation of many different compositions, and an easy incorporation of ions in the crystal lattice. The material, biological, and chemical properties are related to the variation in the electronic structure caused by defects and impurities. Thus, it is necessary to understand the relationship between structural aspects and the material properties upon impurity incorporation [1,2].

The present work is focused on the investigation of Fe-doped hydroxyapatite. In the current study we consider single point defects in several charge states, as it was done in our recent study of the OH vacancy in HAp [3]. The calculations carried out within density functional theory using plane-waves to describe the valence states, and ultra-soft pseudopotentials to account for the core electrons. The generalized gradient approximation to the exchange-correlation accounted for the many-body electronic interactions. The calculated formation energies of defects shows that: 1) Ca(1) and Ca(2) substitutions have almost the same formation energy and are nearly probable. 2) the iron interstitial defects, which are not yet considered in the literature, are even more probable than substitution defects.

References

[1] M.Jiang, J. Terra, A. M. Rossi, M. A. Morales, E. M. Baggio Saitovitch, and D. E. Ellis, *Phys. Rev. B*. **66**, 224107 (2002).
[2] V.Bystrov, *Math. Biol. Bioinform*. **12**, 14 (2017).
[3] L.A. Avakyan, E.V. Paramonova, J. Coutinho, S. Öberg, V.S. Bystrov, and L.A. Bugaev, *J. Chem. Phys.* **148**, 154706 (2018)

O7. Atomic Structure of Multicomponent Metallic Nanoparticles From Extended X-ray Absorption Fine Structure Spectroscopy

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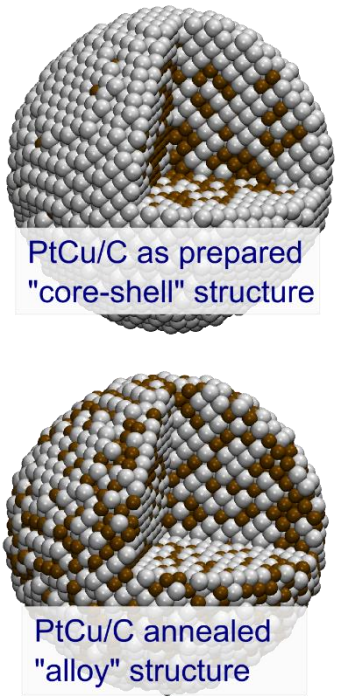
The ongoing increasing of complexity of nanoscale systems requires the improvement of the experimental methods of structure characterization. The extended X-ray absorption fine structure (EXAFS) is a promising method since it is sensitive to local atomic structure and to the chemical species. Moreover, the convenient method of Fourier-transform analysis of EXAFS signal [1] can be augmented by molecular dynamics simulations or even by machine learning techniques [2]. In current study we present the set of techniques used to construct spatial atomistic models of nanoparticles based on EXAFS spectra measured at ESRF and BESSYII facilities of a number of materials: Pt/$Ce_xLa_{1-x}O_{2-\delta}$ [3], PtAg/C [4], PtCu/C [5] (see figure) and Fe/Fe_3C/C. The atomic structure models for these systems are in agreement with available experimental data such as TEM and XRD.



References

[1] C. Lamberti and J. A. van Bokhoven, *X-Ray Absorption and X-Ray Emission Spectroscopy*, John Wiley & Sons, Ltd (2016).
[2] I. Jonane, A. Anspoks, and A. Kuzmin, *Modell. Simul. Mater. Sci. Eng.* **26**, 25004 (2018).
[3] L. A. Avakyan, N. A. Kolpacheva, E. V. Paramonova, J. Singh, U. Hartfelder, J. A. van Bokhoven, and L. A. Bugaev, *J. Phys. Chem. C* **120**, 28057 (2016).
[4] V. V. Pryadchenko, V. V. Srabionyan, E. B. Mikheykina, L. A. Avakyan, V. Y. Murzin, Y. V. Zubavichus, I. Zizak, V. E. Guterman, and L. A. Bugaev, *J. Phys. Chem. C* **119**, 3217 (2015).
[5] V. V. Pryadchenko, V. V. Srabionyan, A. A. Kurzin, N. V. Bulat, D. B. Shemet, L. A. Avakyan, S. V. Belenov, V. A. Volochaev, I. Zizak, V. E. Guterman, and L. A. Bugaev, *Appl. Catal., A* **525**, 226 (2016)

O8. Synthesis and characterization of phosphate glass fibers: mechanical and luminescence properties

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In this study, new phosphate glass fibers doped with rare earth ions such as Europium and Terbium have been developed by melting the phosphate glass and stretch it into thin fibers by monofilament extruder machine to provide fluorescent properties. These materials have attracted great attention because of their unique properties, namely, their lightness of weight, flexibility, and rigidity as well as their high mechanical strength and which they have minimal surface defects compared to the glasses.

Amorphous nature of prepared phosphate glasses was confirmed by X-Ray Diffraction (XRD) and the glass transition temperatures of elaborated phosphate glasses were determined by differential thermal analysis (DTA). Mechanical properties of phosphate glass fibers such as tensile strength and Young's modulus have been studied and the results were evaluated in comparison with previous work [1, 2]. A photoluminescence analysis of the phosphate glasses and the phosphate glass fibers prepared is performed through their emission spectra, absorption spectra, and internal quantum yield.

References

[1] Tan, C., and al., Biomedical Glasses, 4 (1), 57-71 (2018).
[2] Pähler, G., and Rolf B., Journal of Non-Crystalline Solids 49.1-3, 487-496 (1982).

O9. Removal of Methylene Blue Dye by Adsorption Using Alginate–Clay–Activated Carbon nanobiocomposite

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Discharging dyes produced during various industrial activities can be harmful and produce serious environmental problems. Therefore, treatment of wastewater has become one of the major issues in wastewater pollution.

In this work, the preparation and characterization of a composite alginate–clay-activated carbon were investigated for methylene blue (MB) removal from aqueous solution.

The structure and surface characteristics of Alginate-Clay-Activated Carbon composite were analyzed using Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM) while thermal properties were tested using thermogravimetric analysis (TGA).

Adsorption experiments were conducted to examine the effects of adsorbent dosage, pH, time and initial concentration of methylene blue. Conclusively, the bionanocomposte produced can be used as an effective, economic and sustainable adsorbent for removal of MB from aqueous solution

O10. First Principle study on Structural, Electrical, Optical and Mechanical properties of $GaSe_{1-x}S_x$ solid solution (x = 0,0.25,0.5,0.75,1)

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The structural, electronic, optical and mechanical properties of $GaSe_{1-x}S_x$ solid solution (x=0,0.25,0.5,0.75,1) by means of pseudopotential method, employed exactly as implemented in Quantum espresso code was calculated. The electron-electron interaction was treated using generalized gradient approximation (GGA) and local density approximation (LDA) functional. A systematic increase in the band gap with increasing Sulphur concentration in the system was observed. All other physical properties viz. young's modulus, dielectric constant, refractive index etc. was also found to have a systematic change with Sulphur concentration. The results can be used for obtaining a precisely tailored solid solution with desired properties. All results are analyzed and explained.

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O11. A new tolerance analysis approach for deformable assemblies: an industrial case study

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In this article, a new approach of tolerance analysis for deformable assemblies is studied and validated in an industrial environment, the automotive industry as an example. This new approach is based on Method of Influence Coefficients, taking into account the shape defects and the contact between surfaces as well as welding distortion. All these parameters influence the final quality of the assemblies. The comparison between the theoretical and practical study validate the performance of the new approach.

O12. Influence of Niobium additions on sintering behaviors and mechanical properties of injection molded 420 stainless steel powder

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This paper describes the sintering of an injection molded 420 martensitic stainless steel with additions of niobium, with the aim of producing high mechanical properties. And at the same time, microstructural and mechanical characterization of these produced parts was also carried out. At the initial stage, 420 martensitic stainless steel powders were mixed with a multi-component binder system for preparing feedstock. Then the prepared feedstock was granulated and shaped by injection molding. And then, the shaped samples were subjected to the debinding process. These samples were sintered at different temperatures for various times. Samples sintered under the condition that gave way to the highest relative density were heat treated. Sintered and heat treated samples were separately subjected to microstructural and mechanical characterization. All analysis showed that using polymeric binder system led to plentiful martensite ratio and carbide precipitates to be occurred in the injection molded samples. Mechanical characterization was performed by hardness measurements and tensile tests.

References

[1] German, R.M., Bose, A. 1997. Injection Molding of Metals and Ceramics, Metal Powder Industries Federation, Princeton, NJ, 11.
[2] *Davis, J.R., Stainless steels, ASM international, 1994*
[3] *Berrettaa, J.R., Rossib, W., Nevesc, M.D.M., Almeidab, I.A., Junior, N.D.V., Pulsed Nd: YAG laser welding of AISI 304 to AISI 420 stainless steels, Optics and Lasers in Engineering, 45(9), 960-966, 2017*
[4] *Nishiyama, Z., Martensitic transformation. 2012: Elsevier.*
[5] *Nakagawa, H. Miyazaki, T., Effect of retained austenite on the microstructure and mechanical properties of martensitic precipitation hardening stainless steel, Journal of materials science, 34(16), 3901-3908, 1999*
[6] *Bhattacharya, K., Conti, S., Zanzotto, G., Zimmer, J., Crystal symmetry and the reversibility of martensitic transformations, Nature, 428(6978), 55, 2004*
[7] *Coleman, A.J., Murray, K., Kearns, M., Tingskog, T.A., Sanford, B., Gonzalez, E., Properties of MIM AISI 420 via pre-alloyed and master alloy routes, in Proc. 2013 Int. Conf. Powder Metallurgy Particulate Material, Chicago, 2013*

O13. Physical properties of $Fe_{1-x}Cu_x$ films electrodeposited on porous and non-porous silicon

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In this work, $Fe_{1-x}Cu_x$ films were prepared by the electrodeposition method from a sulfate bath with complexing agents under potentiostatic conditions on a both porous and bare silicon substrate at different parameters. The properties of the obtained Fe1-xCux alloys thin films have been investigated. The study was carried out by cyclic voltammetry (CV) and means techniques for the determination of the different properties. The CV measurements showed that the presence of cathodic and anodic peaks associated with deposition and dissolution of Fe1-xCux alloys followed by current increase at more negative potential due to hydrogen evolution reaction. The surface morphology of the FeCu films is analysis using SEM. A high-quality smooth deposit with good substrate adhesion which has been attributed to the reduced oxygen content. A strong dependence of the physical properties with the composition of the thin films is observed. Finally, the thin films produced have been used as anode for lithium batteries.

O14. STUDY THE INFLUENCE OF THE PRE-FINISH GAUGES FORM ON THE EFFECTIVENESS OF THE GROOVES FILLING IN THE FINISHING PASS OF REINFORCING STEEL ROLLING

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During reinforcing steel rolling such geometric defect as the absence of longitudinal or transverse ribs is spread. For a detailed study of the process of reinforcement profile rolling and its further optimization, computer simulation in the software complex DEFORM-3D was carried out. In the works [1-2] the most rational, from the authors' point of view, forms of pre - finishing gauges for rolling of reinforcing steel are proposed - a single-radius oval and a flat oval with double concavity. Also, in the work [3], a new calibration for rolling of round and reinforcing steel was proposed, the main feature of which is the pre-finishing caliber, made in the form of a smooth barrel. To assess the impact of the pre-form gauge on the strain state, a single simulation was conducted, i.e. modeling only the pre-finishing caliber, after which the calculation of the finishing pass was conducted.

From considered calibers, the most uniform distribution of deformation provides a flat oval with double concavity, where the distribution in the vertical and horizontal directions is approximately the same. In the other two calibers, the spread difference is quite different. After rolling in the finishing pass, the metal completely filled the contour of the caliber, as well as the screw incisions of the transverse ribs. The longitudinal ribs are also fully formed. All geometric parameters with tolerances fully comply with the requirements of GOST 10884-94.

References

[1] Smirnov V.K., Shilov V.A., Inatovich Y.V. *Calibration of rolling rolls.* Teplotechnik, Moscow (2010).
[2] Benyakovsky M.A., Bogoyavlensky K.N., Vitkin A.I. *Rolling production technology*. Metallurgy, Moscow (1991).
[3] Asanov V.N., Steblov A.B., Tulupov O.N. *Steel*, Vol. 11, p. 90-92 (2008).

O15. Influence of synthesis parameters on polyamidoxime chelating nanohybrid by radiation induced graft polymerization and emulsion graft polymerization for copper (II) uptake

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Innovative polyamidoxime grafted modified sepiolite nanohybrid has been developed consuming acrylonitrile by two techniques 1-radiation induced graft polymerization (RIGP) and 2-emulsion graft polymerization. In RIGP, the concentration of monomer (acrylonitrile), absorbed dose and dose rate were varied to calculate the maximum grafting yield. The nitrile group in the grafted nanohybrid material was rehabilitated into polyamidoxime. These functional group transformations were recognized by Fourier transform infrared (FT-IR). The morphological investigations and elemental analysis of the developed nanohybrid materials were achieved by FESEM coupled with EDX. XRD study helped in inspecting a decline in percentage crystallinity of the developed polyamidoxime nanohybrid from crystalline pristine sepiolite. Three synthesized polyamidoxime nanohybrids (MS-g-AO5, MS-g-AO7.5, MS-g-AO10) were used to carry out batch adsorption studies for copper uptake. Influence of different aspects like pH, initial concentration, adsorbent dose and time of metal/adsorbent contact was examined and optimized. Pseudo-1st order, pseudo-2nd order and intra-particle-diffusion were employed for kinetic study of removal of copper (II) ion. Equilibrium was accomplished within 30 minutes ensuing pseudo-2nd order model. Two isothermal models (Langmuirian model and Freundlich model) were used to study the adsorption mechanism. The equilibrium process was well demonstrated by Langmuir isotherm model. Adsorption capacity, Qmax, of prepared adsorbents were got in the order of MS-g-AO5> MS-g-AO7.5> MS-g-AO10 with regression coefficient (R^2) values above 0.98 which provides an evidence that the number of active sites for adsorption were correspondingly in the same order. The Qmax was ascertained to be 277.8 mg/g for MS-g-AO5 adsorbent. This study has resulted in the preparation of inexpensive and environmentally harmonious chelating adsorbent to capture copper ion [1-4].

Similar nanocomposites were synthesized by emulsion graft polymerization. The different synthesis factors like concentrations of monomer, initiator and surfactant were studied to obtain maximum grafting yield. Highest grafting (373%) was attained at 1% surfactant, 5% acrylonitrile and 0.1% initiator. After modifying polyacrylonitrile to polyamidoxime, the adsorbent was exposed to adsorption process for the same metal uptake as in the previous study of RIGP. Qmax in this case was found to be 303 mg/g. This illustrates that adsorbent synthesized by this method has more active adsorption sites. The objective of this project was to develop promising nanohybrid possessing the propensity to adsorb selective metals from water/waste water. The ambition was efficiently achieved by both RIGP and emulsion graft polymerization [5].

References

[1] N. García, J. Guzm, and E. Benito, *Langmuir*, 27, 3952–3959, (2011)
[2] Y. Bhardwaj, M. Tamada, Y. C. Nho, M. Nasef, and O. Guven, *Workshop on harmonized radiation graft protocol*, Vienna, IAEA Headquarters, 1-32, (2014)
[3] Y. Xie, J. Wang, and M. Wang, *J.Hazard. Mater*., 297, 66–73, (2015)
[4] H. Chen, Y. Zhao, and A. Wang, *J. Hazard. Mater.*, 149, 346–354, (2007)
[5] F. Huang, Y. Xu, and S. Liao, *Materials*, 6, 969-980, (2013)

O16. Synthesis and characterization of gold nanoparticles immobilized on vinyl modified sepiolite nanofibers

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The use of sepiolite nanofibers as a matrix for procurement of immobilized/supported metal nanoparticles has prospective applications in catalysis and other areas. This study epitomizes the development of gold nanoparticles (GNPs) immobilized on vinyl modified sepiolite (VMS) nanofibers. Gold nanoparticles were synthesized by reducing Au (III) to Au (0) using tri sodium citrate as reducing agent. The formation of gold nanoparticles was confirmed by red coloured hydrosol and a peak at 517 nm by UV-Visible spectrum. The colloidal gold solution contained gold nanoparticles in the size range of 2-3 nm analysed by particle size analyser [1]. The tendency of gold nanoparticles to agglomerate due to their high surface reactivity directs to diminish their ability to perform as an efficient catalyst. This problem can be resolved by immobilizing the discrete gold particles on a suitable support/matrix. Sepiolite is a naturally occurring cost effective nanoclay. Due to unique textural morphology, sepiolite nanofibers have silanol groups on its surface which were utilized to graft hydrolysed vinyl tri ethoxy silane. The grafting was demonstrated by specific vibrations for C-H stretching and bending vibrations characterized by FT-IR spectroscopy. The C-H stretching vibrations (asymmetric and symmetric) were characterised by absorption bands at 2971 and 2882 cm-1 correspondingly while C-H bending vibrations are ascribed by 1390 cm-1 and 1276 cm-l. Zeolitic water vibration at 1660 cm-1 was increased due to the grafting of vinyl group. The gold hydrosol was stirred in appropriate amount of water dispersed VMS for 24 hr. The developed nanocomposite exhibits pink tinge supporting the information given by particle size analyser (2-3 nm). Morphological studies of VMS supported gold nanoparticles were carried out by Field emission Scanning Electron microscopy (FESEM) exhibiting clearly the amalgamation of well dispersed gold nanoparticles. XRD data have revealed that the structural integrity of VMS was retained and peaks at 38˚ (111), 44.7˚ (200), 66.7˚ (220) and 77.6˚ (311) have revealed the adsorption of GNPs on VMS matrix. Immobilized GNPs supported on VMS nanofibers are excellent candidate for catalysis of acetylation of phenols, reduction of 4- nitrophenol to 4-aminophenol and some other reactions [1, 2].

References

[1] M. Chen and H. Kang, ACS *Appl. Mater. Interfaces*, 1-10, (2015).
[2] S. Lateif and S. Grant, *Appl. Clay Sci.*, 53, 236-243, (2011).

O17. Charge Oscillations in PEO from Surface Potential by KPFM

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Purpose

Space charges are seen to be a critical problem in the field of dielectrics and electrical insulations because they can cause a premature electrical breakdown. That is why, both charge build up and decay are necessary to be understood well in detail under biased and unbiased conditions.

Experimental approach

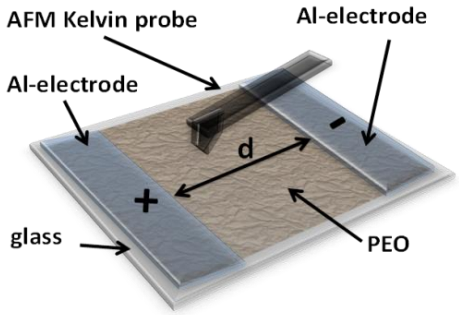

Figure 1 Sample structure

An aluminum-poly(ethylene oxide)-aluminum (Al-PEO-Al) sample structure (see Fig. 1) is used as a model system. Two types of samples, undoped PEO and doped PEO with 0.1%wt lithium percholate, LiClO4, were investigated. The following experimental approach is carried out [1]: First, the surface potential between the electrodes is measured by the Kelvin Probe Force Microscopy (KPFM) under biased and unbiased conditions. Then the measured surface potential is differentiated twice by a reliable statistical smoothing-derivative algorithm with additional feedback loops in order to extract the space charge distribution according to the Poisson equation. The surface potential was measured before, during and after switching off the external voltage.

Results

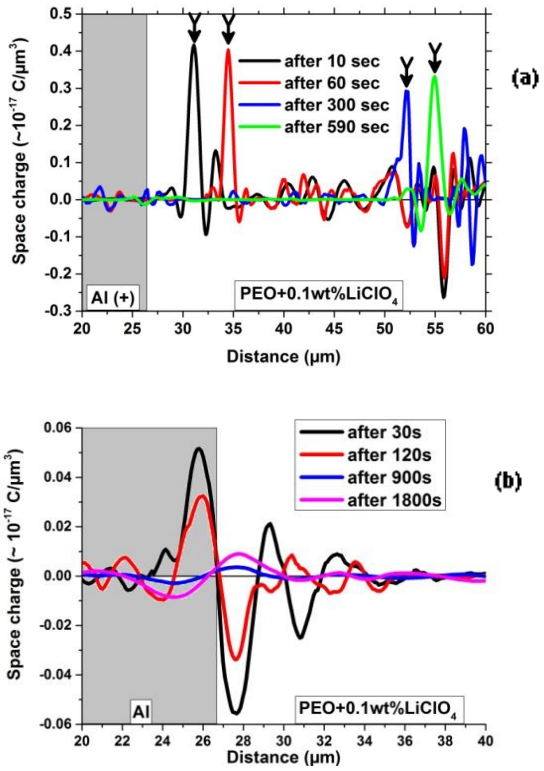

Figure 2 Space charge distributions during the field (E = 0.6MV/m) applied (a) and after switching off the applied field (b)

The space charges were calculated and analyzed for all three situations [2]. Here, for example, we show one of the results. Fig. 2 depicts the space charges at the Al-PEO interface region for the doped sample during and after switching off the applied field E = 0.6 MV/m. The voltage was positive at the left side Al-electrode. A positive charge packet is travelling towards the negative electrode during the field applied. The positions of this charge packet are marked with arrows at four different moments in time (see Fig. 2(a)). In front of this charge packet charge oscillations are found. These charge oscillations inside the PEO are changing in space and time. When the field was applied, negative charges have accumulated in the PEO near the interface. After switching off the applied field, they decrease in time and have turned into positive charges after 900s (see Fig. 2(b)). The induced positive image charges in the Al also decrease and finally turn into negative charges. The charge configuration found 1800s after switching off the field remains constant in time. It results from image forces between ions in the PEO and images in the Al.

Conclusions

The speed of the positive charge packet is higher in the Li-doped PEO than in the undoped PEO. That is because of freely movable positive lithium ions. Dynamic positive and negative space charge regions are identified inside the PEO for the both types of samples. These regions appear as oscillations due to attraction and repulsion processes between positive and negative charges. A three dimensional charge hopping model will be used for the description of this process qualitatively.

[1] K.Faliya, H. Kliem and C. J. Dias, 'Space charge measurements with Kelvin Probe Force Microscopy', IEEE Transactions on Dielectrics and Electrical Insulation, 2017, 24(3), 1913-1922.
[2] K. Faliya, H. Kliem, Charge distributions in poly(ethylene oxide)-based electrolytes for lithium-ion batteries, J. Electrochim. Acta 290 (2018) 211-219.

O18. Photocatalytic degradation of methylene blue under visible light using Cu_2ZnSnS_4 film made of nanoparticle ink

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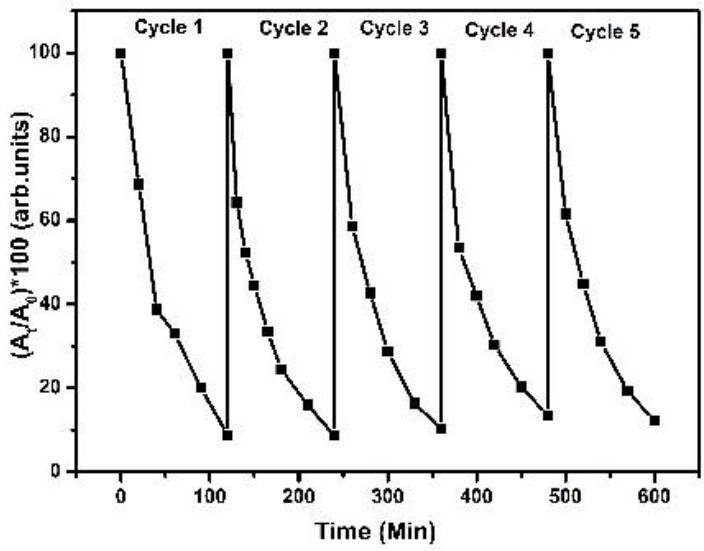
Synthetic dyes are used widely in various industries and degradation of these pollutants is one of the major issues in the concern of environmental safety. Photocatalysis finds application in this context since it could be effectively used for the degradation of dye with the help of light energy. Among the different prospective materials as a catalyst, Cu_2ZnSnS_4(CZTS) has been emerged in the recent years as a potential candidate with which photocatalysis takes place under visible light. Here kesterite structured Cu_2ZnSnS_4(CZTS) is used as a photocatalyst for degradation of methylene blue dye. CZTS nanoparticles with a size of ~ 9 nm is synthesized using wet-chemical methods. An ink of CZTS nanoparticle is made in Toluene and doctor-bladed onto a glass substrate to make a uniform film. The prepared CZTS film has a bandgap of ~ 1.5 eV and is highly suitable for dye degradation under visible light. 60 ml of 0.1mM methylene blue solution with the catalyst is irradiated with 300 W halogen lamp and 90% degradation of dye occurred in an irradiation time of 120 min. 50% of degradation occurred in the first 20 min of irradiation. The apparent first order reaction rate constant is ~ 0.032/min which is higher while comparing with the available visible light photocatalyst at present.

Figure 1. Repeatability study of photodegradation of methylene blue.



The repeatability studies performed for 5 cycles showed a negligible deviation of degradation efficiency upto - 3% from the initial value which proves the suitability of this cost-effective material as a visible light photocatalyst.

O19. Determining the impact of aging on the bacterial toxicity of Zn nanoparticles

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Toxicity of NPs is a new research area that lacks the representation of real environmental conditions. This may result in errors when evaluating the experimental results. In this study we investigated how aging conditions alter the physiochemical structure of NPs and affect its interactions with bacteria. For this purpose, gram negative (*Pseudomonas aeruginosa*) and gram positive (*Staphylococcus aureus*) bacteria were exposed to Zn NPs aged under different conditions. Aging of Zn NPs were accomplished by keeping them in 1%, 10%, and 100% real sea water samples for 1 day and 20 days. Particle size and zeta measurements show that aging NPs for 20 days significantly reduced the size of Zn NPs compared to aging them for 1 day. Furthermore, NPs treated with higher sea water concentration and aged for longer period had higher negative zeta potential values. As reported previously in literature, these physiochemical alterations are ultimately expected to affect the toxic behavior of NPs towards bacteria.

References

[1] X. Lin, J. Li, S. Ma, et al., *PLoS ONE*, **9**, e110247 (2014).
[2] J. Hou, Y. Wu, X. Li, et al., *Chemosphere*, **193**, 852 (2018).
[3] M. Bundchuh, J. Filser, et al., *Environmental Sciences Europe*, **30:6,** (2018).

O20. Mechanical and microstructural investigation of Metakaolin/ phosphate washing sludge Based Geopolymers composites Reinforced with polypropylene fibers

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A large quantity of by-products is generated by the extraction of phosphate ore, which is causing serious problems for the environment[1]. The best approach in overcoming the aforementioned waste management problems is to promote large volume recycling/reuse of these waste materials[2]. The main objective of this study was to investigate the potential reuse of phosphate washing sludge as a partial replacement for metakaolin in the production of geopolymers composites.

After the construction of a metakaolin/phosphate washing sludge(PWS) based geopolymer concrete containing 0.25, 0.5, 0.75,1, 1.5 % of polypropylene (PP) fibers, Compressive strength, flexural strength, water absorption, porosity, thermal conductivity, microstructure and morphology have been characterized and evaluated. The results showed that the optimal strength of a mixed PP-fiber reinforced MK/PWS geopolymer is obtained with 50% of PWS replacement, 0.75% fiber addition and a liquid/solid ratio of 1.21. Also revealed that polypropylene (PP) fibers can enhance mechanical properties in the late age, and shows excellent hardening and strengthening effects on the geopolymer. In addition, SEM results showed that fibers could relieve stress concentration, improve specific surface area and significantly decrease the average pore diameter of the geopolymer.

References:

[1] S. Moukannaa, M. Loutou, M. Benzaazoua, L. Vitola, J. Alami, and R. Hakkou, Journal of Cleaner Production, vol. 185, pp. 891–903, Jun. 2018.
[2] M. M. Al-mashhadani, O. Canpolat, Y. Aygörmez, M. Uysal, and S. Erdem, Construction and Building Materials, vol. 167, pp. 505–513, Apr. 2018.

O21. Crystal growth modes and crystallization kinetics of amorphous films according to transmission electron microscopy "in situ"

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Laser erosion plasma was deposited on substrates of KCl (001) at room temperature. Sputtering of a target (Cr, V, Zr, Hf) was carried out in an oxygen atmosphere ($P(O_2)$ ~ 0.13 Pa) with the use of a radiation from an LTI-PCh-5 laser operating in the Q-switched mode. The thickness of the films varied in the range from 20 to 35 nm. Crystallization of films was initiated by electron beam irradiation in the column of a transmission electron microscope at a beam current of ~ 20 μA. The rate of crystallization was controlled by varying the density *j* of the electron current through the sample, which was varied in the range from 1.1 to 6.5 $A \cdot mm^{-2}$ depending on the electron beam focusing.

The structural analysis was carried out by the methods of electron diffraction and transmission electron microscopy on EM-100L and PEM-100-01 electron microscopes operating at an accelerating voltage of 100 kV. The process of crystallization of a film was recorded from the screen of an electron microscope with a Canon Power Shot G15 camera in the video recording mode at a frame rate of 30 s^{-1}. Data on the kinetics of the crystallization process were obtained from the analysis of individual frames of the video recorded "in situ" at a fixed electron current density.

Electron-microscope investigations "in situ" concerning the crystallization of amorphous films, deposited by laser evaporation, were systematized. Based on the analysis of the structure and morphology of crystals, growing in amorphous films under the influence of an electron beam, the concepts of layer polymorphic crystallization (LPC), island polymorphic crystallization (IPC) and dendrite polymorphic crystallization (DPC) were formed. For each crystallization mode the parameter of dimensionless relative unit of length δ_0, equal to the ratio of the characteristic unit of length to the value, characterizing the size of the unit cell of the crystal, were assigned respectively. Kinetic curves of the dependence of the fraction of the crystalline phase *x* on time *t* were given.

The generality of the processes of crystal growth from the vapor phase on substrate and from the amorphous state in films is that in both cases a disorder-order transition takes place. This predetermines the structural and morphological analogy between the main forms of crystal growth on substrates and the main types of crystallization of amorphous films.

LPC (Cr_2O_3, V_2O_3, Sb_2S_3, Se and others) is regarded as morphological analog of Frank–van der Merwe (FM) growth mode of a crystal from the vapor phase. In the case of LPC in the zone of observation in amorphous film grows a single flat crystal. By analogy with FM growth mode an energy criterion of the LPC can be written as $\sigma_a \geq \sigma_c + \sigma_{ac} + \varepsilon_d$, where σ_a is the free energy of the amorphous phase–vacuum interface, σ_c is the free energy of the crystalline phase–vacuum interface, σ_{ac} is the free energy of the amorphous–crystalline phase interface, and ε_d is the energy of deformation of the growing crystalline layer. For LPS the quadratic dependence of *x* on *t* takes place and δ_0~ 3000-5000.

IPC (Al_2O_3, ZrO_2, Ni, Re and others) is regarded as morphological analog of Volmer–Weber (VW) growth mode of a crystal from the vapor phase. In the case of IPC in the zone of observation in amorphous film grows a lot of small disoriented crystals. By analogy with VW growth mode an energy criterion of the IPC can be written as $\sigma_a \leq \sigma_c + \sigma_{ac} + \varepsilon_d$. For IPS the exponential dependence of *x* on *t* takes place and δ_0~ 100-900.

DPC (HfO_2 and others) is regarded as morphological analog of Stranski–Krastanov (SK) growth mode of a crystal from the vapor phase. A characteristic sign of DPC is the formation of dendrite branches along the sides of a flat single crystal. For DPC the quadratic dependence of *x* on *t* takes place and δ_0~ 3000.

O22. Comparison between linear and nonlinear tolerance analysis of flexible assembly taking into account spot welding effects

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Tolerance analysis for flexible parts and assemblies is the precious step in manufacturing parts industry, in order to minimize the cost of the process the literature have focus the most, in reviewing tolerance analysis for flexible parts and assemblies step. This paper analyses two major methods for tolerance analysis for flexible assembly. Furthermore, to improve the performance of the proposed model that has been simulated to predict the deformation of flexible parts and assemblies, we have taken into consideration the spot-welding effects. Finally, through a comparative study, the results prove the performances of the proposed approach.

O23. Mechanical and microstructural properties of geopolymeric mixtures based on not thermally treated Moroccan phosphate washing sludge: Experimental investigation of new materials as building materials

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From an environmental point of view, a high interest has been given to recycling and valorization of mining by-products to produce valuable products[1, 2, 3].

This work aims at investigating the possibility of reusing Phosphate Washing Sludge (PWS) from phosphate beneficiation plants (Youssoufia, Morocco) to produce eco-friendly building materials through geopolymerization process. In particular, the behavior towards alkali activation process of PWS not thermally heated, in binary mixtures with metakaolin, was evaluated. Mechanical strength, porosity accessible to water were determined after 28 days and the reaction products were characterized by XRD, FTIR and SEM/EDX. Also ATG/DTG tests were performed. Results show an adequate mechanical performance of these materials, with values of the compressive strength as high as 48.97 MPa and low porosity (17.42 %) under room temperature curing, when the content of PWS was more than 50%. In these blends, the sludge acts basically like a filler. However, calcium carbonates present on the sludge (dolomite and calcite) partially dissolve and react in the alkaline mixture favoring the formation of some local high-calcium, high Si/Al ratio (C-A-S-H-type gel) areas co-existing with M-A-S-H-type gel. The use of non-thermally activated PWS represents a valuable complementary approach with reconciling the need of producing reliable building materials towards the development of carbon-free binders.

References

[1] Kinnunen, P., Ismailov, A., Solismaa, & All, M. Journal of Cleaner Production, 174, 634-649 (2018).
[2] Gallala, W., Herchi, F., Ali, I. B., Abbassi, L., Gaied, M. E., & Montacer, M. Procedia Engineering, 138, 85-94 (2016).
[3] Loutou, M., & Hajjaji, Applied Clay Science, 150, 56-62 (2017).

O24. Study of Borophene nanotubes stability and phase transition by molecular dynamics simulation

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Borophene nanotubes were synthesized by thermal reduction of B_2O_3 powder for the first time in 2010 [1]. Theoretical proposals have predicted different structures of Borophene sheets, but experimental studies have revealed that it is a sheet with anisotropic structure and buckling height [2]. In this research, we have simulated the structural stability and phase transition of the Borophene nanotubes by molecular dynamics method and Reax force field. For this purpose, we studied nanotubes with a length of 30 nm and a diameter of 1.21-15 nm for the zigzag and 3.50-15 nm for the armchair nanotubes. The results suggest that the armchair and zigzag nanotubes with the diameters above 4.9 nm and 3.17 nm are stable respectively. Furthermore the Simulation results demonstrated that the Lattice constants along the perimeter of the nanotubes decreases slightly as the diameter increases. Moreover, the cohesive energy of nanotube decreases as the diameter increases indicating more stability. Moreover, we found that the armchair nanotube of 5nm diameter is stable up to about 2110 K and has a cohesive energy and isobaric specific heat capacity about 132 kcal/mol and 29 J/mol.K respectively.

References

[1] F. Liu, C. Shen, Z, Su, et al. J. Mater. Chem. 20, 2197–2205 (2010).
[2] D. A, Mannix, X. F. Zhou, B. Kiraly, et al., Science, 350, 1513-1516 (2015).

O25. Development of repellent surfaces

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Surface contamination is a major industrial problem that leads to significant loss of performance and increased maintenance costs. Numerous methods have been developed to prepare a super-repellent coating but the retention of high levels of repellence has not been achieved yet[1]. The development of surfaces that repel liquids has attracted lots of interest due to variety of possible applications in industry. Whilst there are many examples in the literature of highly repellent and even omniphobic coatings, a deeper understanding of the key chemical and topographic characteristics that dictate this behavior would provide the enabler for the engineering of anti-contamination, anti-sticking and self-cleaning materials[2]. The purpose of this research is to better understand the conditions that dictate very high levels of repellence, specifically to decouple the effect of surface chemistry from surface roughness and to develop a new methodology for assessing wettability.

To deconvolute the effects of surface chemistry from topographic contributions planar glass slides with minimal surface roughness were used as substrates. The surface of these slides were treated with a range of different chemistries known to provide low surface energies[3]. This included silanes, silicones, silazanes and phosphonates, fluorinated and non-fluorinated treatments were included.

Static contact angle measurements were undertaken with both water and diiodomethane, little difference between the various coating types was observed.

Figure 1. Diiodo-methane and water droplets on functionalised planar glass slides

To provide a more discriminating test to enable the selection of the most repellent surface chemistry, an examination of advancing-receding contact angle as a function of tilt from the horizontal has been undertaken. In addition, an evaluation of the droplet location as a function of tilt has been undertaken to determine when the droplet moves and whether it exhibits film-forming behavior.

This approach outlined forms the basis of a new methodology for assessing repellence that accounts for a wider range of behaviours other than simple static sessile drop assessments.

References

[1] A. Wojdyła, G. Durand, A. Taylor, and I. Boyd, Advanced low-energy durable coatings. International Journal of Energy Research, 39(2), pp.165-171 (2014).

[2] C. Hsieh, F. Wu, and W. Chen, Super water- and oil-repellencies from silica-based nanocoatings. Surface and Coatings Technology, 203(22), pp.3377-3384 (2009).

[3] L. Li, B. Li, J. Dong, and J. Zhang, Roles of silanes and silicones in forming superhydrophobic and superoleophobic materials. Journal of Materials Chemistry A, 4(36), pp.13677-13725 (2016).

O26. Thin film functionalization for engineering of biologically active selective sensor surface

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We present the microfabrication of a selective sensing surface for the capture and detection of *Lymantria dispar* (commonly known as gypsy moth) female's pheromone, disparlure[1]. This surface serves as a foundation for the development of a field working sensor, capable of detecting the presence of disparlure and therefore track *L. dispar* females. The latter is of significant importance for isolated ecosystems such as New Zealand, where the introduction of a foreign species could have damaging effects on primary industries.

For the fabrication of the sensing surface we chose a thin gold film patterned with an interdigitated design. These patterned electrodes were functionalized with two specific proteins from *L. dispar* (pheromone binding protein 1 and 2) for the selective capture of the pheromone. The proteins sequence was obtained from the National Center for Biotechnology Information, inserted into a bacterial vector and expressed in an *E. coli* system. The proteins were attached to the gold surface by conjugation with carbon disulfide (CS_2) which adheres to the (111) facet of the gold crystallites and to the protein's N-terminal amine group[3]. To enhance functionalization yield the gold film was annealed to increase the amount of exposed (111) facets[2]. The functionalized electrodes were connected to a potentiostat and Electrochemical Impedance Spectroscopy (EIS) was performed to quantify adhered molecules on the gold surface[4].

Results indicate that the EIS assay is capable of quantifying the amount of adhered material on the surface of the gold electrodes which is signaled by an increase in the impedance component of the EIS signal when protein is attached to the electrodes.

Our work demonstrates the functionalization of thin films for the selective capture and detection of volatile organic compounds (VOC). This same methodology can be modified to fabricate surfaces selective for different molecules, thus overcoming one of the biggest problems with VOC sensors, namely the lack of selectivity and specificity for these types of analytes.

References

[1] E. Plettner et al., Biochemistry, 39(30), 8953-8962 (2000).
[2] Y. Niu, et al., Langmuir, 28(51), 17718-17725, (2012).
[3] C. Nogues et al., Surface Science, 573, L383-L389 (2004).
[4] J. Lazar, et al., Lékař a technika – Clinician and Technology, 45(4), 105-109, (2015)

O27. Nonlinear Optical and Mechanical Features of Conjugated Polymer Nanocomposites

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π-conjugated materials are of great importance in the rapidly growing field of organic electronics due to their unique features upon interaction with light. The reinforcement of such systems with compatible nanoparticles can lead to the generation of novel composite materials with enhanced optoelectronic and mechanical properties. Two nitrophenyl supported poly(1, 3, 4-oxadiazole)s viz; poly[pyridine(2-nitrophenyl)-1, 3, 4-oxadiazole] [PPNO] and poly[2-(*o*-nitrophenyl)-5-phenyl-1, 3, 4-oxadiazole] [PNPPO] were initially synthesized by a dehydrocyclization reaction, and then reinforced with TiO_2 nanoparticles. The nanocomposites have been found to possess charge transfer characteristics from the macromolecular systems (PPNO or PNPPO) to TiO_2 particles, upon photo-excitation. In view of user-friendly device fabrication, flexible films of PPNO and PNPPO were fabricated by blending the composites with 2 wt% of poly(methylmethacylate). The nonlinear optical responses and optical limiting behaviour of PPNO, PNPPO and their nanocomposites were evaluated by Z-scan technique using nanosecond Nd:YAG, 532 nm laser radiations. They possessed strong nonlinear absorption coefficient and a nonlinear refraction coefficient of the order 10^{-10}esu and a third-order nonlinear susceptibility of the order 10^{-11} esu. The nonlinear optical properties of the matrix were found to be enhanced upon TiO_2 loading, as typically attested with the PNPPO/TiO_2 system. Loading of TiO_2 nanoparticles onto polymer matrices has also been found to contribute to a quantum enhancement in tensile properties in the range of 20 MPa-22 MPa. These observations clearly point towards the potential use of TiO_2 loaded PNPPO composites for use in photonic devices and optical switches, and for optical power limiting applications.

References:

[1]. K. Nimisha, E. Shiju, C. Chandrasekar, G. Unnikrishnan, *RSC Adv*. **6**, 115132 (2016).
[2]. W. Xiaoyu, Z. Shuxian, L. Lu, L. Lidong, *ACS Appl. Mater. Interfaces*, **9**, 9051 (2017).

O28. Synthesis of TiO_2-rGO nanocomposites as photocatalysts for the degradation of methylene blue dye in water

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The aim of this study was to synthesize the TiO_2-rGO (titania-reduced graphene oxide) nanocomposites as photocatalysts. The graphene oxide (GO) was synthesized from natural graphite powder by Hummer's method [1]. TiO_2 sol was prepared by using titanium tetraisopropoxide as a precursor, *i*-propanol as a solvent, acetylacetone as a chelating agent and nitric acid as a catalyst [2]. The TiO_2-rGO nanocomposites with different amounts of GO were obtained by a hydrothermal method. They were characterized by means of powder X-ray diffraction analysis, Fourier transform infrared spectroscopy and scanning electron microscopy. The photocatalytic activity of the TiO_2-rGO nanocomposites was evaluated by the photocatalytic degradation of Methylene blue (MB) dye (dissolved in water) as a model pollutant with the irradiation by three different lamps: (I) a light-emitting diode (LED) lamp with a radiation peak at 365 nm, (II) halogen lamp that emits radiation predominantly in visible region and (III) Solar-simulator lamp. The concentrations of MB were monitored by UV-Vis spectrophotometry. Obtained results indicated that photocatalytic properties of prepared TiO_2-rGO nanocomposites depend on the amount of rGO and on the type of the radiation (irradiation source).

References:

[1] D. C. Marcano, D. V. Kosynkin, J. M. Berlin, A. Sinitskii, Z. Sun, A. Slesarev, L. B. Alemany, W. Lu, J. M. Tour, *American Chemical Society Nano*, **4**, 4806-4814 (2010)

[2] L. Ćurković, D. Ljubas, S. Šegota, and I. Bačić, *Journal of Alloys and Compounds*, **604,** 309-316 (2014).

O29. Graphene-Based Porous Adsorbents for CO_2 Capture

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Carbon dioxide global emissions from combustion processes are the main contributor to the observed rising of concentrations of atmospheric CO_2 which causes of global warming and climate change. The strong correlation between atmospheric CO_2 concentration and global climate change has motivated intensive research for the development of cost-effective CO_2 capture processes for the control of CO_2 emissions from coal-fired power plants, the largest single CO_2 source [1].
Adsorption with solid sorbents is one of the most promising options for post combustion (CO_2) capture due to its several advantages over the conventional liquid absorption process such as the minimal amounts of energy required for the capturing technology low energy consumption associated with regeneration, low toxicity of the materials, infinite regenerability, large adsorption capacity, and high stability of the sorbents.
Next generations of CO_2 capture technologies can be achieved by improving the efficiency, reducing the cost of capture and better integration in power generation.
Currently, graphene based porous adsorbents are of great interest because of their porous structure together with the exceptional intrinsic properties of monolayer graphene, nanoporous graphene materials have high specific surface areas and large pore volumes, which ensure a high and rapid adsorption of CO_2.
In this work, functionalized graphene oxide adsorbents were synthesized using amine silane derivatives. Their exhaustive morphological and physical characterization were confirmed by scanning electron microscopy (SEM), small angle X-ray scattering (SAXS), N2 physisorption, and thermogravimetric analysis (TGA).
The CO_2 adsorption capacity of these materials was investigated and the influence of textural properties on the CO_2 uptake studied. CO_2 diffusion can be accelerated by more amine sites exposed and accessible for CO_2 sorption. As a result, the sorption capacity increases at a temperature of 25 °C and a pressure of ~1 atm.

References

[1] Kenarsari, S. D.; Yang, D.; Jiang, G.; Zhang, S.; Wang, J.; Russell, A. G.; Wei, Q.; Fan, M. Review of Recent Advances in Carbon Dioxide Separation and Capture. RSC Adv. 2013, 3, 22739.

O30. Surface modification of polyethylenimine coated magnetic nanoparticles in water treatment

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In recent years, nanoscience and technology has introduced a new dimension to scientific disciplines and technology sectors due to its ability to exhibit superfunctional properties of materials at nano-dimensions. There is a remarkable rise in research and development in all developed countries and many developing countries pertaining to this field.

Magnetic nanoparticle (MNP) is a new kind of nanometer-sized material and widely used in biotechnology, biomedicine fields and as efficient adsorbent with large specific surface area and small diffusion resistance. Among the magnetic nanosized materials, metal oxides like iron oxide (magnetite, Fe_3O_4 and maghemite, γ-Fe_2O_3) play a major role in many areas of sciences. Recent advances in their synthesis give access to size controlled, monodisperse particle. In addition to convenient magnetic properties and low toxicity and cost, MNPs exhibit high surface to volume ratios, depending on the particle size, which associate to their ability for surface chemical modification, can show enhanced capacity for uptake in water treatment procedures [1]. However, an unavoidable problem associated with particles in this size range is their intrinsic instability over longer periods of time. Such small particles tend to form agglomerates to reduce the energy associated with the high surface area to volume ratio of the nanosized particles. Moreover, naked metallic nanoparticles are chemically highly active, and are easily oxidized in air, resulting generally in loss of magnetism and dispersibility. For many applications it is thus crucial to develop protection strategies to chemically stabilize the naked magnetic nanoparticles against degradation during or after the synthesis. Therefore, a suitable coating is essential to overcome such limitations.

Magnetic nanoparticles were synthesized by hydrolysis method. MNPs were coated with polyethylenimine onto the surface of the MNPs following the reported procedure**.** The surface of MNPs-PEI was modified with various functionlized moieties thiosalicylic acid, 2-thiophene carboxaldehyde, orthovanillin and EDTA. The synthesized nanomaterials materials were characterized by FT-IR, TGA, XRD, HRSEM amd HR-TEM. The adsorption capacity of the synthesized nanoabsorbents for lead was evaluated. The optimized conditions for higher absorption at room temperature were found to be at pH 6.5 and 10mg of absorbent for 100 ml of solution of 25ppm Pb^{2+}.

References

[1] R.C. Peña, L. Cornejo, M Bertottic, Desalination and Water Treatment 84 (2017) 271–278

O31. Organo functionalised core shell magnetic nanomaterial as adsorbent for aqueous heavy metals removal

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Water demand has increased as a consequence of different human activities and industrial growth. Water pollution is a worldwide problem due it being incapable of biodegradation and are thus persistent in the environment. Therefore, it is necessary to develop new methods and materials for removing contaminants from wastewater.

Nanomaterials reveal good result than other techniques used in water treatment because of its high surface area and activated functionalized sites. Technologies based on the utilization of magnetite nanoparticles for the removal of heavy metals from wastewaters are under active development as highly effective, efficient and economically viable nanoadsorbents. Among the main advantages of these nanomaterials is the possibility of surface modifications with different organic or inorganic coating agents to allow the removal of a wide range of heavy metals with specificity. However, there is much recent interest in using of engineered magnetite nanoparticle in wastewater treatment. In this work further step was taken in the application of magnetic nanoparticles on solid support as highly efficient, recoverable, stable, and cost-effective catalyst which prepared by environmentally friendly procedure. We synthesize organo functionalised magnetic nanoparticles on solid support for the removal of heavy metal cations in waste water. It is applied as an efficient and economical adsorbent for green removal of lead(II) ions from water. A core-shell magnetic nanostructure was prepared by performing hydrolysis in alkaline solutions using tetraethylorthosilicate (TEOS) and functionalising the silica coating with a terminal linker which was further modified with different organic molecules for further increase in the catalytic selectivity towards cations.

The process of modifying was confirmed by HR-SEM, HR-TEM, ATR-IR spectroscopy and X-ray diffraction. Structural studies showed that the Fe_3O_4 core were cubical in shape with a uniform mesoporous shell. The structural integrity of the materials was not comprised during the surface modification.

It is applied as an efficient and economical adsorbent for green removal of lead(II) ions from water. Magnetic nanoparticles were strongly influenced by an external magnetic field and resulted in the separation from the aqueous media within 1 minute. To its adsorption capabilities, the effect of dosage of adsorbent, contact time, initial pH and initial concentration of lead ion are scrutinized. Owing to high adsorption capacity of these catalysts, lead ion can be removed considerably, up to 80%, and the adsorption reaches equilibrium within 10 min under optimized conditions. Regeneration and reusability of these catalysts were able to regenerate without significant adsorption capacity loss.

References

1. J. Wilcox (Ed.) Carbon Capture, 2012, springer, New York.

O32. Femtosecond laser processing of Ag/CdS doped oxide glasses

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Femtosecond laser processing (FLP) of Ag/CdS doped oxide glasses opens new routes for precise 3D space-selective tuning of material properties and precipitation of luminescent Ag clusters, CdS quantum dots or plasmonic Ag nanoparticles [1, 2]. Such laser processing of glass is of particular interest for the development of optical data storage and integrated photonics waveguides. Hence it is crucial to understand processes which take place during the FLP including local chemical composition change, influence of glass matrix and laser parameters on the FLP. In this work we performed FLP of zinc phosphate and silicate glasses doped with Ag and CdS using high power near IR femtosecond laser system PHAROS SP coupled with 3D Aerotech translation stage. We demonstrate the possibility of simultaneous formation of luminescent silver clusters and plasmonic silver nanoparticles in phosphate glasses as well as of luminescent CdS quantum dots in silicate glasses spatially confined in micron-sized pipe-shaped domains inside glass. We show that laser treatment induces micro-modification of optical properties manifested in the appearance of luminescence and absorption in the visible spectral range and homogeneous birefringence in the laser-exposed domains. Using energy dispersive X-ray spectroscopy, we showed Ag ions migration process from center to the boundary of domains as well as migration of Zn to the center. Ability to form complex 3D shapes of luminescent, plasmonic and birefringent structures embedded in dielectric transparent glass materials will pave the way for the design of nanophotonic devices and multilevel optical memory. This study was financially supported by the Russian Foundation for Basic Research (grant 18-33-00595 and 19-32-80032).

References

[1] Shakhgildyan G.Yu. et al., *J. Non-Cryst. Solids*, **Volume 481**, Page 634-642 (2018).
[2] Vetchinnikov M.P. et al., *Opt. Lett.*, **Volume 43**, Page 2519-2522 (2018).

O33. DNA-noble metal nanoparticles complexes for biomedical applications

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Nanoparticles of precious metals, in particular, gold and silver, have unique physical and chemical properties that allow them to be used for biomedical purposes [1]. They can be used as drug transport agents and in biocatalysis. In addition, surface plasmon resonance is observed in metallic nanoparticles, which allows them to be used as a marker and to enhance Raman scattering.

Gold nanoparticles (AuNPs) are widely used in different areas because of their unique properties. Efficiency of usage may vary with the size and shape of particles which depends on synthesis. A new method of creating very stable gold nanoparticles in solutions containing chloroauric acid or its salt and synthetic copolymer without reducing agent is proposed. The optimal concentrations of components and the exposure time for obtaining homogeneous gold nanoparticles were selected. The formation of compact DNA-copolymer complexes with the inclusion of these AuNPs was viewed.

The fabrication of nanoparticles was controlled by spectrophotometry and viscometry. The size and shape of AuNPs and compact DNA structures were obtained from the dynamic light scattering, atomic force microscopy and scanning electron microscopy data.

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References

[1] A. Kumar, S. Kim, and J.-M. Nam, *JACS*, **138**, 14509-14525 (2016).

O34. Local Electric-Field Induced Phase and Domain Transformations in (1-x)$BiFeO_3$-$BaTiO_3$ systems

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Searching of lead-free materials with the electromechanical characteristics comparable to lead zirconate titanate is an actual topic during recent decades due to the increasing demands of ecology in production and recycling. Bismuth ferrite (BFO) possesses large polarization which is indicative of possible efficient electromechanical performance [1]. The main problem of BFO material is poor phase stability and high leakage current [2]. To improve phase stability and realize morphotropic phase boundary (MPB) conditions, different strategies can be used. As example, doping by rare earth elements leads to formation of rhombohedral and orthorhombic phase coexistence, while solid solution of BFO with barium titanate tends to develop into pseudocubic lattice symmetry. BFO-based materials realizing MPB conditions are prospective to improve piezoelectric properties by means of extrinsic contribution from domain walls' and phase boundaries' movement in electric field.

Here we focus on local-scale studies of the phase coexistence in BFO-based solid solution with different structural compositions: rhombohedral, orthorhombic and pseudocubic. We demonstrated X-ray diffraction to show only average symmetry of solid solutions correspondent to the non-polar lattice ordering. In the same time, local study by piezoresponse force microscopy with nanoscale resolution approves clustering of polar phase. Local transformation of phases was shown to be part of polarization reversal process. Thus, PFM-based studies of phase composition, domain and phase field-induced dynamics are crucial for comprehensive characterization of BFO-based solid solutions.

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References

[1] Fujino S., Murakami M., et al., *Appl. Phys. Lett.*, **92**, 202904 (2008).
[2] Walker J., Bryant P., et al., *Acta Mater.*, **83**, 149 (2015).

O35. Sizing Electrode and its effect on performance of a microactuator

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The vibration amplitude and its frequency are the main factors that affect the performance of resonating microactuators and microsensorson. Electrostatic and piezoelectric actuation/sensing are very common methods used to design Microelectromechanical Systems (MEMS). Both methods requires adding electrode layer for detection or actuation purposes which is normally vey small is dimension and therefore have low effect on the performance of MEMS device. In some cases, small shift in the vibration resonance frequency of the device or its amplitude of vibration can highly affect the device performance. This work investigates the effect of sizing electrode on the performance of electrostatically actuated MEMS device. Electrode length was varied from fully covering the actuator layer to covering 10% only. ANSYS finite element was used as a simulation tool.

References

1- Amer Abdallah, Ali Ishag, Salah El-Deen Osman, Mohanad Yousif, and Musaab Hassan, “Thermal Analysis of Electrostatic Micro Actuator”, International Journal of Mechatronics, Electrical and Computer Technology, Vol.4(10), 2014
2- Ammar Atia, Moayad Mamoon Ibrahim, Omer Abd Algbar Mohamed and Musaab Hassan, “Modeling Of Electrostatically Actuated Temperature Sensor”, International Conference on Computing, Electrical and Electronics Engineering, Corinthia Hotel, Khartoum, 26 Aug - 28 Aug 2013
3- Brissaud, M., Ledren, S., & Gonnard, P. (2003). Modelling of a cantilever non-symmetric piezoelectric bimorph. JOURNAL OF MICROMECHANICS AND MICROENGINEERING, 13(6), 832–844.
4- Kuang, J.-H., & Chen, C.-J. (2005). The nonlinear electrostatic behavior for shaped electrode actuators. International Journal of Mechanical Sciences, 47(8), 1172–1190.
5- Yuan, Y., Du, H., Xia, X., & Wong, Y. (2014). Analytical solutions to flexural vibration of slender piezoelectric multilayer cantilevers. SMART MATERIALS AND STRUCTURES, 23(9)
6- Lee, C.-C., Guo, Q., Cao, G. Z., & Shen, I. Y. (2008). Effect of electrode size and silicon residue on piezoelectric thin-film membrane actuators. Sensors and Actuators A: Physical, 147(1), 279–285.
7- Ghayesh, M. H., Farokhi, H., & Alici, G. (2015). Size-dependent electro-elasto-mechanics of MEMS with initially curved deformable electrodes. International Journal of Mechanical Sciences, 103, 247–264.
8- Nadim Maluf , Kirt Williams ,"An Introduction to Microelectromechanical Systems Engineering", Second Edition,2004

O36. STM lithography at MoO_2/Mo(110) surface

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STM is a proper tool to produce a remarkable modification of the surface under investigation. It can result in atom evaporation [1], initiation of chemical reactions [2], etc. Both inelastic tunneling and strong electric field in a STM tip – surface gap contribute into modification of the surface. Scanning Tunnelling Microscopy (STM) is a useful tool for the analysis of the surface of many conducting materials which possess atomic resolution. However, atom manipulation is one of exciting options of STM. We have used STM to study surface modification and separate contribution of tunneling current from electric field generated by a probe of STM.

A monolayer of extra oxygen atoms was prepared by exposition of MoO_2/Mo(110) surface in oxygen ($P=10^{-7}$Torr) at room temperature [3]. STM experiments demonstrated that extra oxygen can be removed from the surface top layer solely by means of electric field generated by STM tip. Despite of a smooth distribution of electric field it was possible to remove individual extra oxygen atoms from the surface. However, tunneling current increases the probability of oxygen atom to be escaped. We have proposed a models of surface modification both by tunneling current and electric field generated by a probe of STM. This has been confirmed by DFT simulations.

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1. Baptiste Gault, Michael P. Moody, Julie M. Cairney, and Simon P. Ringer. Atom probe microscopy. Springer Series in Materials Science, 2012.
2. H. J. Kreuzer, Physics and chemistry in high electric fields, Surface and Interface Analysis 2004; 372–379 Published online in Wiley Inter Science
3. Krasnikov, S.A., Lübben, O., Murphy, B.E. et al. Writing with atoms: Oxygen adatoms on the MoO2/Mo(110) surface, Nano Res. (2013) 6: 929

O37. Reconfigurable Metamaterial Perfect Absorber

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Metamaterials (MMs) as electromagnetic illustrative with artificial operations can get attained by configuring on the sub-wavelength scale.[1] Because the resonant optical characteristics of plasmonic MMs depends on the near-field dielectric circumstances, they specify a vigorous and an adjustable substitute for metals. Although various MMs has been introduced with a representative reflection to induced stimuli such as light and electric field, but the majority of them showed volatile switching state.[2, 3] To overcome this bottleneck, we integrated a phase change metamaterial (PCM) in the nanophotonic device structure. We take benefits from the loss elements of the optical constant (real components) to establish an elevated absorber. A near-zero reflectivity is achieved by controlling the μ and ε resonances and matching MM impedance to the free space.[4, 5] Metamaterial-based programmable perfect absorber (MPA) is a reconfigurable device with an absorbance near unity. It has been shown that optically- stimulated PCM specifies a non-volatile MM modulator of transmission and reflection for near- infrared (NIR) to mid-infrared (MIR) wavelengths with a subwavelength thickness.[2] Our design consists of three main layers in a simple metal-insulator-metal (MIM) structure including a dielectric thin film (spacer) which is sandwiched between two metallic layers. The structure is analogous with Fabry-Perot (FP) etalon with an ultrathin cavity according to the top electrode (TE) arrayed nanoparticles. TE is a patterned metallic layer which conveys an electric reply relevant to the grounded bottom electrode (BE) by intensely coupling to the electric field at a specific resonance frequency.[1]

References

1. Watts, C.M., X. Liu, and W.J. Padilla, "Metamaterial electromagnetic wave absorbers", Advanced materials, Vol. 24, No. 23, 98-120, 2012.
2. Gholipour, B., et al., "An all-optical, non-volatile, bidirectional, phase-change meta-switch", Advanced Materials, Vol. 25, No. 22, 3050-3054, 2013.
3. Driscoll, T., et al., "Memory metamaterials", Science, Vol. 325, No. 5947, 1518-1521, 2009.
4. Hedayati, M.K., F. Faupel, and M. Elbahri, "Review of plasmonic nanocomposite metamaterial absorber", Materials, Vol. 7, No. 2, 1221-1248, 2014.
5. Landy, N.I., et al., "Perfect metamaterial absorber", Physical review letters, Vol. 100, No. 20, 207402, 2008.

O38. Structural Studies of Metal-Organic Frameworks for Selective Adsorption of Hazardous Contaminants from Aqueous Solutions

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The steady increase in global population along with continued economic development is contributing in deterioration of clean water supply. The continuous release of contaminants such as dyes, pesticides, heavy metals, pharmaceuticals, etc. in water can disturb the aquatic surroundings. Therefore, removal of these contaminants from water has become significantly important to reduce the threat of environmental pollution. Due to remarkable advancement in modern material technology, significant efforts have been devoted to develop novel nanoadsorbents for the removal of these contaminants from aqueous solutions. Among various adsorbents, metal-organic frameworks (MOFs) are the most promising functional nanomaterials due to their large surface area, high degree of porosity, and tuneable structure-property relations. Here, we have combined the benefits of porous MOFs matrix and functional properties of encapsulated nanoparticles for efficient removal of these hazardous contaminants (i.e., pesticides). The successful green synthesis of MOFs and their nanocomposites were characterized by several spectroscopic and microscopic techniques such as UV-Vis, FTIR, FESEM, XRD, BET, TGA, etc. These nanocomposites are found to be effective adsorbents with due consideration of different performance parameters such as pH and adsorbent/adsorbate dose.

References

[1] M. Nehra, N. Dilbaghi, N.K. Singhal, A.A. Hassan, K.H. Kim, and S. Kumar, *Environmental research*, **169**, 229-236 (2019).

[2] S. Alhan, M. Nehra, N. Dilbaghi, N.K. Singhal, K.H. Kim KH, and S. Kumar, *Environmental Research*, **173**, 411-418 (2019).

O39. Proton conductivity in BCY10 in nominally dry conditions

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Electrochemical membrane reactors using proton-conducting ceramics are promising and efficient technologies for the production of valuable chemical products by the promotion of hydrogenation/dehydrogenation reactions [1]. Due to a very high equilibrium constant for hydration, yttrium-doped barium cerate, $BaCe_{0.9}Y_{0.1}O_{3-\delta}$ (BCY10) presents one of the highest proton conductivities at low temperatures of the known proton-conducting ceramic oxides (*e.g.* ~10^{-3} S cm^{-1} at 400 °C under humidified atmospheres, p_{H2O} ~ 10^{-2} atm) [2]. Nonetheless, BCY10 is commonly discarded for such applications due to its poor chemical stability towards hydroxide or carbonate formation [3]. Moreover, the use of humidified atmospheres may not be feasible for many chemical syntheses, due to undesired side reactions.

The current work, therefore, combines impedance spectroscopy, thermogravimetric analysis, coulometric titration and defect chemistry modelling to assess the limits for pure protonic conductivity in BCY10 in nominally dry atmospheres (p_{H2O} ~10^{-4}-10^{-5} atm, at low temperatures < 600 °C); conditions where its stability and applicability to industrially relevant chemical synthesis reactions may be maintained, whilst still being hydrated. This work, thereby, unlocks a new application area for proton-conducting ceramics to a wide range of hydrogenation/de-hydrogenation reactions in the nominal absence of water.

References

[1] Morejudo, S. H. *et al.*, *Science*, 353, LP-566 (2016).
[2] Kreuer, K. D., *Annu. Rev. Mater. Res.*, 33, 333–359 (2003).
[3] Fabbri, E., Pergolesi, D. & Traversa, E., *Chem. Soc. Rev.*, 39, 4355–4369 (2010).

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O40. Synthesis and characterization of Ni/rGO nanocomposite: from nickel nanoclusters to homogeneously distributed discrete nickel nanoparticles

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Graphene oxide (GO) has been investigated as a substrate for the controlled growth of different type of nanoparticles (NPs) allowing to develop new multifunctional nanocomposites with high performance for different applications [1]. Among inorganic NPs, Ni NPs have been the focus of intense research due to its remarkable conductive [2], catalytic [3] and hydrogen storage [4] properties. However, accurate control of nanocomposite's structure is needed to improve final properties. Here we present a two-step synthesis protocol based on a solvothermal method, supplemented by a thermal treatment under H_2 atmosphere, to decorate reduced graphene oxide (rGO) with nanosized Ni nanoparticles (NPs). The solvothermal reaction time showed to be a crucial experimental parameter for the control of Ni NPs size and density at rGO surface. At the initial stage of the reaction, it was observed that GO surface is saturated by the nucleation of Ni nanoclusters. Over the reaction time, GO began to reduce, and the adjacent nanoclusters were able to diffuse and coalesce at the rGO surface, forming monodispersed ultrafine Ni NPs. A subsequent thermal treatment under reductive H_2 atmosphere formed crystalline Ni/NiO core-shell structure NPs on rGO surface. This nanostructured Ni/GO hybrid materials can find interesting applications in different areas, namely nanoelectronics and energy storage technologies.

References

[1] M. Khan et al., J. Mater. Chem. A, 3, 18753 (2015).
[2] F. Bidault et al., Int. J. Hydrogen Energy, 34, 6799 (2009).
[3] W. Zhang et al., Sci. Rep., 5, 10589 (2015).
[4] C. Zhou et al., ACS Appl. Mater. Interfaces, **8**, 15232 (2016).

O41. Free vibration investigation of single walled carbon nanotubes with rotary inertia

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In this study, the authors presented a computational structural dynamic analysis based on Eringen's elastic constitutive model [1]. Single walled carbon nanotubes SWCNTs are the subject of this study to investigate their transverse flexural free vibration first resting in an elastic medium, second as a rotating cantilever SWCNT and then as a nanorotor based SWCNTs (figure.1).

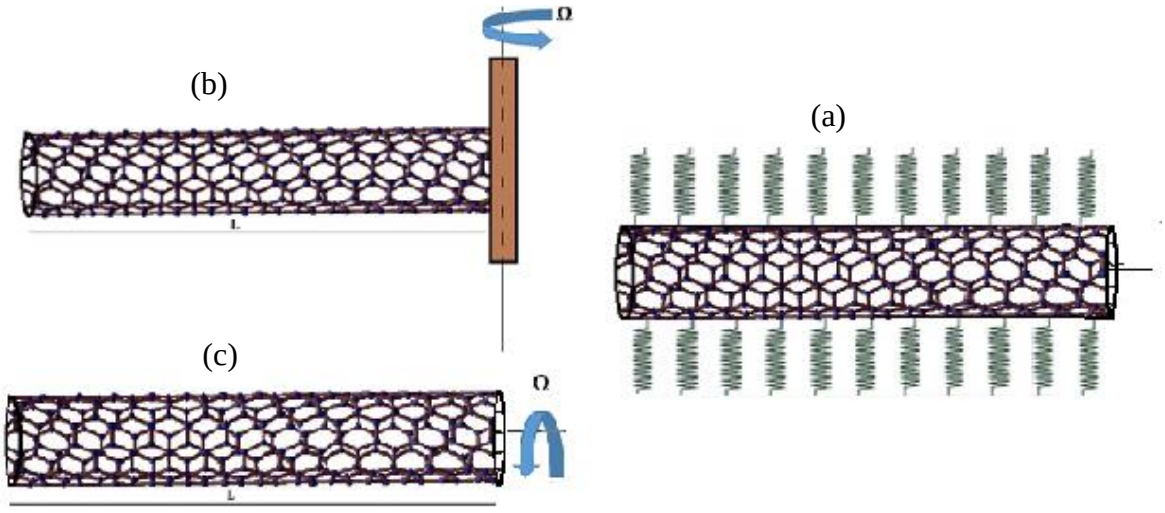

Figure.1 Studied SWCNT configurations: (a) SWCNT embedded in an elastic medium. (b) SWCNT as a rotating cantilever beam. (c) SWCNT as a nanorotor.

Governing equations of motion are derived via Hamilton principle that employed the virtual works to combine between kinetic, strain and potential equations. Generalized differential quadrature method (GDQM) [2] is employed to discretize and resolve the Eigen problem, it is a semi analytic technique based on Lagrange polynomial interpolation to compute derivatives of a function as a sum of weighting coefficients. Boundary conditions of involved in this study are: simply supported beam (S-S), simply supported-clamped beam (S-C)and bi-clamped beam (C-C)
The discretization and the resolution of governing equations of motion that are derived based on Hamilton principles, is worked out by using the semi-analytical technique, generalized differential quadrature method (GDQM) that is highly recommended for structural nanomechanical problems.

The effect of small scale, boundary conditions and angular velocity on the dynamic parameters is studied. results obtained from this study are summarized as following:

- At nanoscale, nonlocal elasticity with other non-classical elastic theories are employed to model the problem.
- CNT's offer exceptional mechanical properties that are highly required in nanotechnology applications, in particularly next generation rotating nano-machinery

• For SWCNT resting in elastic foundations, the elastic medium decreases their frequency parameters.
• For rotating cantilever nanobeam, angular velocity parameter increases the fundamental frequency parameter, so the nonlocal parameter does for fundamental frequency. A high order mode of vibration inversed the effect of nonlocal parameter.
• For the SWCNT nanorotor [3], Rotary inertia of the SWCNT nanostructure have split the frequency parameter to forward and backward frequencies (Campbell diagram).
• The increased 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.

References

[1] A.C. Eringen, *J. Appl. Phys*. **54**, 4703 (1983).
[2] R. Bellman, B.G. Kashef, J. Casti, *J. Comput. Phys*. **10**, 40 (1972).
[3] A. Belhadj,A. Boukhalfa, and S. A. Bellia, Eur. Phys. J. Plus, **132**. 513 (2017).

Poster presentations

P1. XPS, FTIR and photoelectron emission spectroscopies to analyze nanocapacitor silicon nitride nano layered structures

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Dielectric Si_3N_4 nanolayers (SNN) are widely in use for nanocapacitors. To reach high electrical capacitance, thin SNN are required. The minimal thickness of SNN is limited due to their inhomogeneity. To avoid this, SNN are assembled from nano-multilayers. However, their optimal number is unknown.

The purpose of this study was to identify an influence of the SNN number on quality of the nanocapacitors (NC).

The SNN were fabricated because of the low-pressure chemical vapor deposition.

The supplied multilayered structures were characterized due to XPS, FTIR and photoelectron emission spectroscopies. Electrical properties of NC originated from SNN were measured as well.

The following main results have been achieved:
- the minima of the oxygen concentration appeared at the SNN interfaces;
- the 500-470 cm^{-1} absorption minimum shift was induced by the SNN number;
- the photoelectron emission maxima intensity depended on the SNN number;
- the breakdown voltage of NC was increased with the number of the multilayers.

The above demonstrated that electrically active centers were delivered by the SNN boundaries.

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P2. Ferroelectric domain wall motion in lead-free BST thin films

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$Ba_{0.8}Sr_{0.2}TiO_3$ (BST) thin films with a thickness 400 nm were prepared on Si substrates by the RF magnetron sputtering. We have investigated the nanoscale domain growth dynamics of ferroelectric BST thin films using piezoresponse force microscopy (PFM) on both as-grown and prepoling surface [1]. The nanoscale domains of dot patterns were formed by applying voltage pulses to the PFM tip. The domain radius was linearly proportional to logarithmic value of the pulse width. The observed difference between the linear sizes of the domains formed at different signs of electric field is associated with the influence of interface effects on propagation of polarization under the cantilever. Also, the obtained activation field (activation fields of wall motion for positive and negative voltage pulses could be obtained to be 3.4×10^7 and 4.1×10^7 V/m) was in the same order with ferroelectric oxides. This asymmetry in activation field is correlated with the pinning state of the films. Therefore, the BST film with good polarization switching properties could act as a memory element in nonvolatile ferroelectric random access memory (NV-FRAM) devices.

The study was supported in part by the Russian Foundation for Basic Researches (project 18-29-11029).

References

[1] D.A. Kiselev, M.S. Afanasiev, S.A. Levashov, G.V. Chucheva, "Growth kinetics of the induced domains in ferroelectric BST 80/20 thin films". *Phys. Solid State*, **57**, 1151-1154 (2015).

P3. Development of magnetic nanoparticles for use in conjunction with radiofrequency heating for greener processes

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With the increasing demand to develop greener processes, the use of non-traditional energy sources particularly in the form of electromagnetic radiation has gained much attention recently as it presents a more effective method of heating in contrast to conventional forms of heating. In addition, the integration of magnetic properties in the catalyst not only allows for a simple magnetic separation but also heat to be generated within the catalyst bed under an alternating magnetic field. Heating through these mechanisms facilitates a uniform temperature profile across the reactor which limits formations of hotspots and thermal runaway which can create by-products and waste. Also, the small distance for heat transfer from the magnetic core to the catalytic surface avoids resistances and increases energy efficiency.

This research investigates magnetic catalysts and their applications that are of significance in the organic, fine chemicals and pharmaceutical sectors. A relevant reaction is hydroalkenylation which is a class of C-C bond forming reactions between alkenes to yield branched alkenes. This reaction is particularly of interest as its products are formed in a more efficient manner in terms of atom economy. Also, hydroalkenylation is complementary to the olefin cross metathesis reaction which received a Nobel prize in 2005. Therefore, exploration of this reaction is relatively new in comparison to the many reactions that have already been carried out using RF heating and magnetic catalysts. [1]

This project concentrates on hydroalkenylation involving styrene and related compounds which has been homogeneously tested. [2] There has been no record of any heterogenization and no attempt to immobilize the traditional compounds used at all, let alone any effort to integrate these compounds with magnetic nanoparticles. In this research, this is achieved by synthesis of nanoscale core-shell materials and includes optimization of catalytic parameters and characterization of properties of the material to maximize heat generation and various selectivities. The reaction is typically carried out in batch mode, thus converting it to a continuous flow configuration is rather novel. The use of continuous flow and internal heat generation is able to successfully address challenges presented in this reaction such as the slow reaction rate and high catalyst loading required.

The synthesis of novel materials presented here has great potential to tackle common concerns that arise during the design stage of a process. As the reactor is the center of a process, optimization of this stage is of significance as it has a direct impact on the subsequent operations such as the product purification, recovery and treatment, which can not only contribute a large proportion of the final product cost, but also produce harmful waste and end up being energy intensive which may ultimately lead to increased emissions.

[1] T. Houlding, P. Gao, V. Degirmenci, K. Tchabanenko and E. Rebrov, *Materials Science and Engineering: B*, **193**, 175-180 (2015).
[2] J. Dai, J. Wu, G. Zhao and W. Dai, *Chemistry - A European Journal*, **17**, 8290-8293 (2011).

P4. Optimizing Citral-loaded Lipid Nanoparticles using a 2^2 Experimental Factorial Design

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INTRODUCTION

Citral, commonly known as lemon grass, corresponds in weight to 70 % to 85 % of the essential oil of *Cymbopogon citratus*. Citral is widely used in cosmetics, in food industry as a flavor additive and in the production of vitamin A. The current literature assigns to citral a broad spectrum of therapeutic activities, such as anti-inflammatory, antimicrobial and anticancer. The high volatility of its monoterpenic molecules decreases its pharmacological efficacy. This study aimed to develop and optimize the encapsulation of citral in solid lipid nanoparticles (SLN) by a 2-level experimental factorial design.

MATERIALS AND METHODS

Imwitor 900K was used as a solid lipid containing 40 % to 55 % of monoglycerides. Kolliphor P188 was used as a surfactant. Citral was the starting material. SLN dispersions were produced by dispersing the lipid phase, composed of citral and Imwitor 900K in an aqueous solution of Poloxamer 188 using the hot high-pressure homogenization (HPH) technique. The established dependent variables - mean particle size (Z-Ave), polydispersity index (PDI) - were both analyzed by dynamic light scattering (DLS), and zeta potential (ZP) assessed by electrophoretic light scattering. The influence of the independent variables, surfactant ratio (Poloxamer 188) and lipid ratio on linalool-loaded SLN characteristics was evaluated using a 2^2 factorial design. The dependent variables were Z-Ave, PDI and ZP. For each factor, the lower and higher values of the lower and upper levels were represented by (-1) and (+1), respectively. The central point was replicated three times for estimating the experimental error and represented by (0). The data were analyzed by STATISTICA 7.0 software.

RESULTS AND DISCUSSION

The Z-Ave varied from 97.7±1.2 nm to 441.1±143.6 nm, whereas the PDI ranged from 0.221±0.006 to 0.519±0.027. ZP was approximately zero (mV) in all formulations due to the non-ionic nature of the surfactant. For each of the three dependent variables, analysis of the variance (ANOVA) was conducted with a confidence level of 95% (α= 0.05). No statistical evidence (*p*-value > 0.05) was reported indicating that the variation and interaction between the Imwitor 900K and Poloxamer 188 does not affect the outcome of dependent variables of SLN-citral.

CONCLUSIONS

According to the obtained results, the optimal SLN dispersion consisted on the central established point composed of 1.0 % of citral, 4.0 % of Imwitor 900K and 2.0 % of Poloxamer 188. These results are expected to lead to an efficient lipid nanoformulation enhancing the therapeutic activity of citral, which is currently being studied through *in vitro* assays.

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References

1. L Hagvall, J Brared Christensson. 2014. *Contact Dermatitis*. **71(5)**:280-288.

2. Y Bhalla, VK Gupta, V Jaitak. 2013. *J Sci Food Agric*. **93(15)**:3643-3653.

3. SL Pereira, AM Marques, RT Sudo, MAC Kaplan, G Zapata-Sudo. 2013. *Molecules*. **18(3)**:3072-3085.

4. J Marcus, ML Klossek, D Tourand, W Kunz. 2013. *Flavour Fragrance J*. **28(5)**:294-299.

P5. Lipid Nanomaterials for the Targeting of Triamcinolone Acetonide to Retinal Müller Cells *in vitro*

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INTRODUCTION

Macular degeneration is one of the leading causes of vision loss amongst millions of human beings all over the world presenting increased prevalence due to the world population ageing. Nowadays, attention is devoted to the development of effective systems for the delivery of ophthalmic medicines. The aim of this study was to assess the outcome from the interactions between loaded triamcinolone-acetonide (TA) and the lipid matrix on the uptake profile of TA-NLC by retinal Müller cells performed *in vitro*.

MATERIALS AND METHODS

Nanostructured lipid carriers (NLC) were produced as described by Araujo *et al*. The lipid phase, composed of a mixture of 6.3% (m/m) Precirol ATO5, 2.7% (m/m) squalene, 0.2% (m/V) monolein and 0.025% (m/m) triamcinolone acetonide, and the aqueous phase - composed of 1.8% (m/V) of Lutrol F68 - were heated up to 80ºC separately. The lipid phase was then dispersed in the aqueous phase under high-speed stirring, using Ultra Turrax T-10 for 30 seconds at 7,000 rpm, to form a pre-emulsion which was then passed (3 cycles/600 bar) through a high-pressure homogenizer, obtaining an oil-in-water (O/W) nanoemulsion which was cooled down to 4ºC to allow the recrystallization of the lipid phase and the formation of NLC dispersions. HPLC was used for the quantification of the loaded TA. For the uptake studies, TA was replaced by rhodamine B (RhB). For quality control purposes, particles were characterized regarding their mean particle size (Z-Ave), polydispersity index (PDI), surface charge, and morphology. Cell studies were carried out in rabbit retinal Müller (glial) cells. Müller cells were treated with TA-NLC after enzymatic isolation from adult retinae and phagocytosis was monitored either by transmission electron microscopy (for TA-NLC) or by fluorescence microscopy (for RhB-NLC).

RESULTS AND DISCUSSION

TA-NLC of mean size 159.7±1.3 nm, polydispersity index (PI) 0.16 and zeta potential -43.2 mV were yielded. Encapsulation efficiency higher than 95% was reached immediately after production. Müller cells are responsible for retinal structure and function, while selective cell destruction causes retinal dysplasia, photoreceptor apoptosis and, at a later stage,

retinal degeneration. The development of site-specific carriers for *in situ* delivery of steroids is reasoned also by the fact that the osmotic swelling may also be induced by inflammatory mediators. Retinal glial cells *in vitro* exhibited phagocytotic activity over Precirol/squalene-based NLC, both loaded with TA or with RhB.

CONCLUSIONS

Our study clearly demonstrates that cell-cell interactions play a relevant effect on the nanoparticles' clearance from the cell lines. Precirol/squalene-based NLC loading triamcinolone acetonide are promising carriers for the treatment of retinal edema. Additional studies are currently ongoing to test the effect of NLC surface on their targeting properties.

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References

1. J. Araujo, M.L. Garcia, M. Mallandrich, E.B. Souto, A.C. Calpena. Release profile and transscleral permeation of triamcinolone acetonide loaded nanostructured lipid carriers (TA-NLC): in vitro and ex vivo studies. *Nanomedicine: nanotechnology, biology, and medicine*. 8 (2012) 1034-1041.

2. J. Araujo, E. Gonzalez-Mira, M.A. Egea, M.L. Garcia, E.B. Souto. Optimization and physicochemical characterization of a triamcinolone acetonide-loaded NLC for ocular antiangiogenic applications. *International Journal of Pharmaceutics.* 393 (2010) 167-175.

3. J. Araujo, S. Nikolic, M.A. Egea, E.B. Souto, M.L. Garcia. Nanostructured lipid carriers for triamcinolone acetonide delivery to the posterior segment of the eye. *Colloids and surfaces*. B, Biointerfaces, 88 (2011) 150-157.

4. J.F. Fangueiro, F. Veiga, A.M. Silva, E.B. Souto. Ocular Drug Delivery - New Strategies for Targeting Anterior and Posterior Segments of the Eye. *Current pharmaceutical design.* 22 (2016) 1135-1146.

5. E. Souto, J. Fangueiro, R. Müller. Solid Lipid Nanoparticles (SLN™), in: I.F. Uchegbu, A.G. Schätzlein, W.P. Cheng, A. Lalatsa (Eds.) *Fundamentals of Pharmaceutical Nanoscience*. Springer New York (2013), pp. 91-116.

6. A. Reichenbach, A. Wurm, T. Pannicke, I. Iandiev, P. Wiedemann, A. Bringmann. Müller cells as players in retinal degeneration and edema, *Graefe's archive for clinical and experimental ophthalmology = Albrecht von Graefes Archiv fur klinische und experimentelle Ophthalmologie*. 245 (2007) 627-636.

P6. Di- and tetrasubstituted double-decker silsesquioxanes as building blocks for molecular and macromolecular frameworks

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Polyhedral Silsesquioxanes are a wide class of organic-inorganic, i.e. hybrid compounds, containing well defined nanosized, 3D inorganic core of Si-O-Si bonds and organic coronae.[1] The scientific interest in these systems has now turned to a specific type of frameworks, i.e. double-decker silsesquioxanes (DDSQ), that is reflected in the literature by reports on the synthesis of their molecular and macromolecular DDSQ-based derivatives, representing two major trends in the development and understanding of their interesting physicochemical properties.[2] Herein a synthetic methodology and application of *i.a.* di(dimethyl)vinylsiloxy-(DDSQ-2OSi-Vi) and tetra(dimethyl)vinylsiloxy-(DDSQ-4OSi-Vi) silsesquioxanes with different organosilicon spacer is presented. Using the optimized conditions for hydrosilylation reaction, we are presenting a procedure for efficient formation of co-polymers with DDSQ-based derivatives that were isolated and characterized by Gel Permeation Chromatography, spectroscopic and thermal methods.

References

[1] D. B. Cordes, P. D. Lickiss, F. Rataboul, *Chem. Rev.* **110**, 2081-2083 (2010)
[2] B. Dudziec, B. Marciniec, *Curr. Org. Chem.* **21**, 2794-2813, (2017)

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P7. SYNTHESIS OF NANOSTRUCTURES AND FILMS USING HIGH-TEMPERATURE VACUUM ELECTRIC FURNACE

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The need for extensive research on the synthesis of carbide silicon and diamond-like films requires the creation of an economical vacuum electric resistance furnace, which allows to reach temperatures up to 1400 °C and above [1,2]. A low-inertia and economical vacuum high-temperature graphite resistance furnace with geometrical dimensions of cylindrical working area of 125 mm of height and diameter of Ø33 mm, has been developed and manufactured. The furnace increases a temperature above 1400 °C for no more than 120 minutes and capable of synthesizing amorphous and crystalline SiC and diamond-like films in the atmosphere of CO, methane and other gases. The furnace is equipped with 6 screens – two cylindrical graphite reflectors of 1.5 mm thick with a smooth and polished surface, as well as cylindrical reflectors of tantalum and stainless steel. Graphite heater, sapphire tube and graphite reflectors are designed in a single unit. The high-vacuum chamber is designed to obtain a vacuum of 10^{-2}–10^{-4} Pa. Graphite heaters have been manufactured and tested. The temperature of 1427°C has been achieved at the power of 3318 W. The electrical resistance of the heater during heating decreased from 2.45 to 1.35 Ohms.

Heat treatments of SiC films have been conducted. An annealing in a high-temperature furnace of thick amorphous silicon carbide films deposited by magnetron sputtering in a high-frequency mode of 13.56 MHz on the c-Si surface under the following conditions was carried out: the deposition time was 18000 s; the magnetron power - 150 W, the argon gas consumption - 2.4 l / h, the chamber pressure - 0.4 Pa, the substrate temperature - 100°C. The formation of thick amorphous and nanocrystalline films of silicon carbide is shown by IR spectroscopy and X-ray diffraction. It is shown that after deposition, more than half (54.9%) of Si–C-bonds are found in very small nanoparticles with sizes less than 3 nm, the formation of which can be interpreted by exposure to a high-frequency field. Annealing of thick SiC films on Si substrates in a developed and manufactured high-temperature furnace at a temperature of 1100°C for 30 minutes led to an improvement in the structure of the film, the formation of SiC nanocrystals with a tetrahedral bond. The low-temperature formation of α-SiC may be due to the influence of the high-frequency (13.56 MHz) mode of the magnetron sputtering used while simultaneously sputtering silicon and graphite targets.

An influence of annealing in vacuum at the temperature of 720°C on the formation of $TiSi_x$ structural phases in Ti-Si system is also considered. The mutual diffusion of Si and Ti atoms, the formation of Ti and $TiSi_2$ nanocrystals, are analyzed.

References

[1] S.A.Kukushkin, K.Kh.Nussupov, A.V.Osipov, N.B.Beisenkhanov, D.I.Bakranova. Structural properties and parameters of epitaxial silicon carbide films, grown by atomic substitution on the high-resistance (111) oriented silicon. Superlattices and Microstructures. 111. 2017. P.899-911.

[2] Marmer E.N. High-temperature technologies and electric furnaces for heat treatment and sintering. // International scientific journal Alternative Energy and Ecology. 1 (69). 2009. p. 14-49.

P8. The structures of non-IPR isomers 29 (C_2), 31 (C_s), 38 (D_2) and 39 (D_{5d}) of fullerenes C_{40}

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The lower fullerenes C_n (n<60) are highly unstable due to large strain energy and the violation of the isolated pentagon rule (IPR), making them extremely hard to study experimentally. So, considering an experimental breakthrough in the preparation of such fullerene as exohedral derivative [1], the purpose of this theoretical investigations is test of the approach developed early by us [2] to lower fullerenes to establish possibility of they production. In this report, we investigated the molecular structures of non-IPR isomers 29 (C_2), 31 (C_s), 38 (D_2) and 39 (D_{5d}) of fullerene C_{40}.

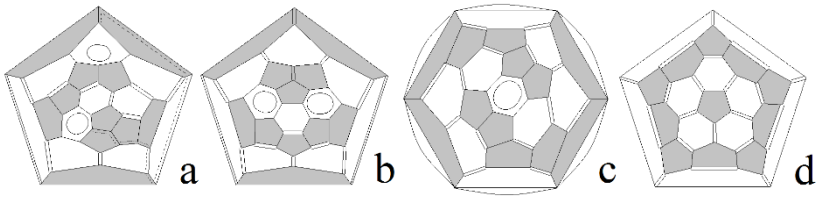

Figure 1. Schlegel diagram of isomers 29 (C_2) (a), 31 (C_s) (b), 38 (D_2) (c) and 39 (D_{5d}) (d) of fullerene C_{40}.

Quantum chemical calculations (DFT) show that isomers 31 (C_s), 38 (D_2) and 39 (D_{5d}) have a closed electronic shell, whereas isomer 29 (C_2) has an open-shell structure. The data about the distributions of single, double and delocalized π-bonds in researched isomer molecules are presented for the first time as well as their molecular formulas (figure 1). The preliminary bonds distributions according to developed approach are confirmed in DFT calculations. It is found that partial π-bonds delocalization and chain of such delocalized bonds passing through some cycles are appeared. Identified features in the structure of lower fullerene molecules can be predictive of the ability to their synthesis as derivatives.

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References

[1] S.Y. Xie, et al, *Science*, **304**, 699 (2004).
[2] A.R. Khamatgalimov, and V.I. Kovalenko, *Russ. Chem. Rev.*, **85**, 836 (2016).

P9. Ythrene: Radical Fullerene Substructure in Fullerenes Molecules

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Among higher fullerenes that obey the isolated pentagon rule (IPR) there are appreciable share of fullerenes with open electron shells. For the long time this rule was used as a criterion for fullerene stability. Notwithstanding the IPR, fullerene radicals are unstable as pristine fullerenes but may be stabilized as their derivatives. Mainly, the molecules of such fullerenes contain phenalenyl radical substructures. Here for the first time we found and theoretically investigated a new radical substructure of fullerene molecules of IPR isomer 7 (C_{3v}) of C_{82} that bears two unpaired electrons and of IPR isomer 822 (D_{3d}) of C_{104} with two equivalent substructures (four unpaired electrons).

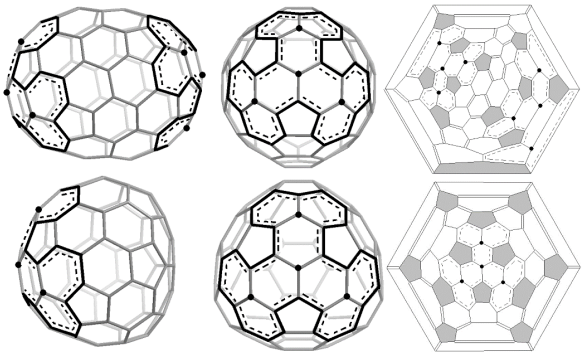

Figure 1. 3D (two views) and Schlegel diagrams of the IPR fullerene molecules: C_{104}, isomer 822 (D_{3d}) (top), and C_{82}, isomer 7 (C_{3v}) (bottom).

According to our computations, two hypothetical polyaromatic radical molecules $C_{34}H_{18}$ and $C_{34}H_{12}$, which are the models of the fullerene substructure, have the same open-shell triplet ground states..

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P10. Titanium oxide-peroxide as a precursor for preparing titania coatings

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Recently we have found that annealing of the $[TiO_x(O_2)_{2-x}(H_2O)_m]$ phase produced by treating titanyl sulfate with various peroxo compounds (hydrogen peroxide, ammonium persulfate, or urea hydrogen peroxide) results in formation of titanium dioxide [1]. The purpose of the work was to use the $[TiO_x(O_2)_{2-x}(H_2O)_m]$ phase for preparing coatings on glass and aluminum.

Coatings on glass were prepared by deposition of the polymeric titanium complex containing urea and/or peroxo bridging ligands followed by annealing. Coatings on aluminum were prepared by anodizing an aluminum sample in the solution containing 20% H_2SO_4, 5% glycerin, 5% lactic acid, and $[TiO_x(O_2)_{2-x}(H_2O)_m]$ (0.125 A/cm^2, 10–15 min).

The resulting coatings were characterized by X-ray diffraction and IR spectroscopy. They demonstrate good mechanical properties and chemical stability. Thin films containing nanocrystalline anatase show high photocatalytic activity in the model reaction of Methyl Orangs discoloration. Therefore, $[TiO_x(O_2)_{2-x}(H_2O)_m]$ is a promising precursor for manufacturing nanostructured thin-film coatings.

References

[1] E.V. Savinkina, L.N. Obolenskaya, G.M. Kuzmicheva, I.D. Morozov, and R.G. Chumakov, *J. Mater. Res.*, **33**, 1422 (2018).

P11. Influence of Structure and Aggregation State of Silver-Gold Nanoparticles on Optical Extinction Spectra

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Gold and silver nanoparticles are of great interest due to their linear and nonlinear optical properties, such as the surface plasmon resonance (SPR) [1]. These properties are depend on the distribution of components in bimetallic Au-Ag nanoparticles, varied from core-shell to alloyed structures [2]. However, the agglomeration of nanoparticles also alters the spectra [3].

In current study we consider the optical spectra of Ag-Au nanoparticles synthesized in glass matrix using Ar-F laser irradiation with energy below ablation threshold [4]. The layered or alloyed nanoparticle structure effects, as well as influence of agglomeration, are studied by T-matrix approach [5] using developed MSTM-STUDIO [3] software.

It is shown that nanocomposites structure heavily depends on the number laser pulses and the energy of first pulse. After 10 laser pulses the Au-core Ag-shell nanoparticles are formed, while bigger number of pulses lead to the diffusion of components and to alloyed particles formation. The importance of nanoparticles agglomeration is discussed.

References

[1] D. J. de Aberasturi, A. B. Serrano-Montes, and L. M. Liz-Marzán, *Advanced Optical Materials* **3**, 602 (2015).
[2] A. V. Skidanenko, L. A. Avakyan, E. A. Kozinkina, and L. A. Bugaev, *Phys. Solid State* **60**, 2571 (2018).
[3] L. A. Avakyan, M. Heinz, A. V. Skidanenko, K. A. Yablunovskiy, J. Ihlemann, J. Meinertz, C. Patzig, M. Dubiel, and L. A. Bugaev, *J. Phys.: Condens. Matter* **30**, 45901 (2017).
[4] M. Heinz, V. V. Srabionyan, L. A. Avakyan, A. L. Bugaev, A. V. Skidanenko, S. Y. Kaptelinin, J. Ihlemann, J. Meinertz, C. Patzig, M. Dubiel, and L. A. Bugaev, *J. Alloys Compd*. **767**, 1253 (2018).
[5] D. W. Mackowski and M. I. Mishchenko, *J. Quant. Spectrosc. Radiat. Transfer* **112**, 2182 (2011).

P12. First-principles investigation of structural, magnetic and optoelectronic properties of Mn and Gd doped zinc blende CdS

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To understanding the effects of rare earth and transition metals on the II-VI semiconductors the structural, magnetic and optoelectronic properties of Mn and Gd-doped zinc blende CdS are investigated extensively and compared with undoped CdS using the first principle calculation. We find that the Mn doped CdS has a semiconducting character as well as the undoped CdS. While the Gd doped CdS has a half metallic character with a high spin polarization at the Fermi level with an important magnetic moment which makes it promising material for spintronic applications. Furthermore, the calculated optical properties of all simples attain its maximum in the visible region and ultra-violet region which make theme suitable for solar cells.

Table 1: Structural parameters of undoped CdS, CdS:Mn and CdS:Gd.

	a(A°)	B(GPa)	B'
CdS	5.9343 (5.78)[2]	53.2814	4.8783
CdS :Mn	5.9176	53.7708	4.7350
CdS :Gd	5.9851 (5.73)[2]	51.5353	4.4346

Table 2: The calculated band gap for spin up and spin down (eV) the available experimental data and others calculated results.

	Eg_{up}	Eg_{Ddn}	Exp
CdS	1.012	1.0029	2.42[2]
CdS:Mn	0.928 (0.65)[1]	1.224 (1.33)[1]	
CdS:Gd	1.56	-	2.96[2]

References

[1] D.E. Aimouch, S. Meskine, A. Birsan, V. Kuncser, A. Zaoui, A. Boukortt, *Materials Chemistry and Physics*,(2018).
[2] Gajanan Pandey, Supriya Dixit, A.K. Shrivastava, *Materials Science and Engineering* B 200 (2015) 59–66

P13. A new family of alkynylsubstituted silsesquioxanes

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Catalytic transformations have become one of the most powerful tool for the synthesis of functionalized organosilicon compounds, also silsesquioxanes. They are a specific frameworks with rigid inorganic Si-O-Si core and reactive and/or inert organic coronae.[1] Silylative coupling, among others, have gained a lot of interest as useful reaction for modification of organosilicons and silsesquioxanes.[2, 3]

In this presentation, we demonstrate an efficient and selective route for "the marriage" of these two issues, i.e. silylative coupling with the ethynylsubstituted silsesquioxanes that gives a new class of silsesquioxane-based systems with silylalkynyl functionality and Si-O-Si core in one molecule.[4] These new compounds possess interesting physical and chemical properties that affect their potential applications.

References

[1] Editor: C. Hartmann-Thompson, Applications of Polyhedral Oligomeric Silsesquioxanes, Springer Netherlands, 2011.
[2] B. Marciniec, B. Dudziec, I. Kownacki, Angew. Chem., Int. Ed., 45, 8180 (2006).
[3] B. Dudziec and B. Marciniec, Curr. Org. Chem., 28, 2794 (2017)
[4] K. Zmudzińska, M. Rzonsowska and B. Dudziec (in preparation)

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P14. Single source precursor synthetic route to quaternary chalcogenide Cu_2FeSnS_4 nanocrystals as potential solar energy materials

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Up to now range of methods have been reported for the synthesis of Cu_2FeSnS_4 NCs of different shapes and sizes.[1-3] The hot injection method is the most commonly used method for synthesis of size selective QDs with controlled shape and reproducibility. The method often use organic capping agents such as trioctylphosphine (TOP), oleylamine (OA) and other long chain amines, which increase the complexity of reaction, causes impurity in the products and enhances the toxicity of NCs. Therefore, it is mandatory to have an alternative facile approach for synthesis of CFTS NCs. The melt method utilized in the present study has many advantages and has been used to prepare CFTS nanocrystals in large quantities in the lab. The technique is a straight forward, inexpensive and single step utilizing xanthates as single source precursors for the fabrication of CFTS NCs. Phase pure quaternary chalcogenide nanocrystals of Cu_2FeSnS_4 from Sn(II) and Sn(IV) have been synthesized using solvent-less, simple and inexpensive melt method using a mixture of Cu^{2+}, Fe^{3+}, Sn^{2+} and Sn^{4+} O-ethylxanthates and annealed at different temperatures. The as-synthesized nanocrystals were characterized by (p-XRD), Raman spectroscopy, UV–Vis absorption, scanning electron microscopy (SEM) and energy dispersive X-ray (EDS). The average particle size of the nanocrystals calculated using Scherrer's formula was found to be 13 nm each for both synthesised. Optical measurements show that the Cu_2FeSnS_4 nanocrystals which have synthesised from Sn(II) and Sn(IV) exhibit strong visible light absorption with direct band gap values of 1.35 eV and 1.37 eV, suitable for photovoltaic applications.

References

1. C. Yan, C. Huang, J. Yang, F. Liu, J. Liu, Y. Lai, J. Li, Y. Liu, *Chem. Commun*., **48,** 2603-2605 (2012).
2. X. Jiang, W. Xu, R. Tan, W. Song, *J. Chen, Mater. Lett.*, **39**, 102-103 (2013).
3. Ai LH, Jiang, *J. Mater Chem.*, **22**, 20586–20592 (2012).

P15. Synthesis of maleic anhydride copolymer catalyzed by maghnite-H+

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Green chemistry aims to design products and chemical process that reduce or eliminate the use and synthesis of hazardous substances. We performed the copolymer synthesis of maleic anhydride with vinyl acetate catalyzed by maghnite H + under environmentally friendly conditions.
This copolymer is characterized, confirmed by transformation of IR quencher, H + NMR nuclear magnetic resonance, 13C NMR, DSC.

References

[1]Metzger, J. O. Angew. Chem. Int. Ed., **37**, 2975-2978**,** 1998.
[2] Schwaiz, J. A. Chem. Rev. **95**, 475-488, 1995.

P16. Micro- and nanohardness of gallium sulfide crystals

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Gallium sulfide and gallium selenide crystals are semiconductor optical materials efficiently used in laser IR optics and in non-linear optics as frequency converters. In this view their mechanical properties are crucial for all applications. Since these materials are brittle and have propensity to exfoliation, it is difficult to study mechanical characteristics using traditional techniques. This was incentive to apply nanoindentation to GaS and to compare the results with microindentation. In this work we also used a melt growth technique, X-ray diffraction, light microscopy, scanning electron microscopy and atomic-force microscopy. Single crystals of β-GaS were grown from melt. Oliver and Pharr method [1] was used for the first time to get mechanical characteristics of nanoindentation. Hardness of micro- and nanoindentation of GaS crystals was found to depend on load. A difference between nano- and microhardness at the same loads is explained by different ways stress is applied to a sample: continuous in the case of nanoindentation and impact for microindentation. At loads higher than 0.2 N the indentation technique and Oliver and Pharr method are not reliable for measuring hardness of GaS crystals, because pile-ups and cracks form upon indentation.

References

[1] W. C. Oliver, G. M. Pharr, J. Mater. Res., **vol. 7,** no. 6, pp. 1564-1584 (1992).

P17. Basal cell carcinoma-targeted therapy using aptamer functionalized liposomes

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The objective of the present study was to obtain a new formulation based on aptamer-functionalized liposomes for delivery of 5-fluorouracil (5-FU), as an anticancer drug widely used in the treatment of BCC. To obtain the liposomes functionalized with AS1411, thiol-terminated AS1411 was conjugated to liposomes via the formation of a thioether linkage. Aptamer conjugation increased liposome size, suggesting that the presence of an additional hydrophilic molecule on the liposomal surface increased the hydrodynamic radius. As expected, the negatively charged DNA aptamer reduced the surface potential of the liposomes. The drug encapsulation efficiency was between 6.8 and 8.7%. Vertical Franz diffusion cells with artificial membranes were used to evaluate the *in vitro* release of 5-FU. The average cumulative amount released per unit area from the formulations was proportional to the loading efficiency. The *in vitro* cell viability, *in vitro* targeting capability and apoptotic effects of aptamer functionalized liposomes on the human dermal fibroblasts cell line (HDF), used as model cell, were also evaluated. The results obtained were satisfactory and will be the basis for new tests to prove the effectiveness of these formulations in the treatment of BCC.

Acknowledgement

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P18. Aptamer-Functionalized Polymeric Nanocapsules — a promising alternative for the Basal Cell Carcinoma treatment

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New type of nanocapsules based on chitosan carboxylate functionalized with AS1411 aptamer and poly (N-vinylpyrrolidone-*alt*-itaconic anhydride) loaded with 5-Fluorouracil were developed, with the potential to improve the treatment of basal cell carcinoma. Functionalization of nanocapsules with AS1411 aptamer will enhance their recognition by tumor cells, due to the interaction with nucleolin, and subsequent endocytosis. Nanocapsules were prepared by interfacial condensation method in the absence of any toxic crosslinking agents. The nanocapsules diameter varied between 100–267 nm. SEM images revealed that nanocapsules were spherical and presented relatively low dimensional polydispersity. The release efficiency of 5-Fluorouracil was studied, the processes being controlled by the drug diffusion through the polymeric membrane, as confirmed by the theoretical analysis of drug release. The cytotoxicity and hemolysis tests performed on the nanocapsules proved their lack of toxicity and their excellent hemocompatibility.

Acknowledgements

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P19. Synthesis and Structural Characterization of Erbium Electrodepositing on Silicon nanowires

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In this work, we report the electrochemical deposition of Erbium on silicon nanowires array (SiNWs). The silicon nanowires were elaborated by metal assisted chemical etching and the Erbium was electrodeposited by two methods, Chronoamperometry and pulsed, then this was followed by a high temperature annealing step.
We used several means of characterizations. We started, first, with the presentation of MEB, EDX, and DRX characterization.
Figure 1 shows DRX spectrum, We found several peaks positioned at 2θ= 20.33°, 41.60°, 56.40°, 60.64° and 80.71° to cubic (space group Ia3) phase Er2O3 according to the PDF 77-777, exhibit an intensity increase for doping pulzed during 40s.
The results presented in this paper indicate that erbium doped silicon nanowires can be useful towards developing efficient and economical devices using these materials.

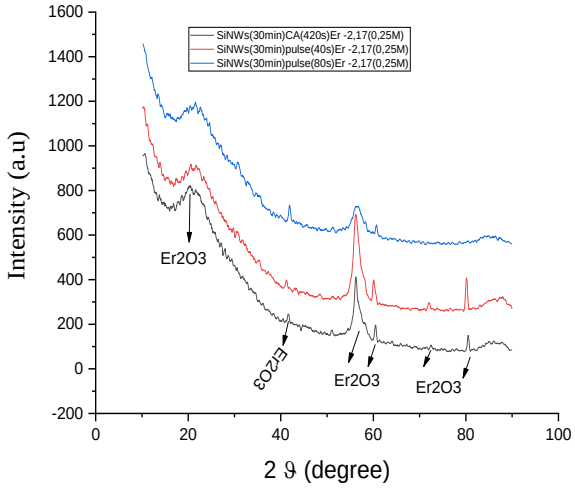

Figure.1: Diffractogram RX of a layer of silicon nanowires with electrodeposited erbium from 0.25M concentration solution (-2.17 potential)

P20. Influence of the magnetic field on the structure and properties of epoxy composites with metal oxides

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This work is devoted to the study of the effect of external permanent magnetic field on the structure, thermophysical, dielectric properties of epoxy polymers and their composites containing metal oxides (CdO, PbO, Cr_2O_3). Samples of composites were formed from epoxy resin ED-20 and triethylenetetramine. Stoichiometric ratio was 1 mole of epoxy resin to 0,18 mole triethylenetetramine. Powder CdO, PbO and Cr_2O_3 were used as fillers. The content of metal oxide was 3 vol. %. The influence of constant magnetic field was $2 \cdot 10^5$ A/m. All curing processes were done at 293 – 297 K for 24 hours. Then all polymeric samples were carried out temperature stabilization at 333 ± 2 K for 24 hours. System studies of structure, thermophysical, thermomechanical and dielectric properties of composites filled with diamagnetic or paramagnetic metal oxides formed under the influence of external constant physical field were carried out for the first time. Patterns of connection between the structure and the physical and mechanical properties of epoxy composites were first established.

The introduction of inorganic filler causes the epoxy polymer to dissolution of the structure and reduces the glass transition temperature of the epoxy composite. The estimation of the influence of constant physical fields on the tangent angle of the dielectric losses of the filled composites shows that the orientation effect of constant physical fields increases the free volume of molecular chains of the chemical network of the epoxy polymer.

References

[1] Ю. В. Бардадим, В. О. Віленський, Вплив фізичних полів на теплофізичні і діелектричні властивості епоксидних композитів, *Фізика і хімія твердого тіла,* **4**, 533 – 539 (2016).

[2] Yu. Bardadym, E. Sporyagin, The influence of the constant physical fields on structure of polymer composites with cadmium oxide and polyaniline, *62nd International Conference for Students of Physics and Natural Sciences «Open Readings 2019»*, 19 – 22 March, Vilnius, Lithuania, 325 (2019).

P21. Minimization of the concentration quenching effect of Tris(bipyridine)ruthenium(II) chloride dye

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The goal of our investigation is to minimize the concentration quenching (CQ) effect which is influenced on the luminescent fluorophores and limited their effectiveness and, consequently, the range of application. Tris(bipyridine)ruthenium(II) chloride (RuBpy) is also known as a photostable dye which is used for chemical and biological research [1–3]. The main disadvantage of this dye is the low fluorescence emission, which drops significantly when the limiting concentration is reached, above which CQ is observed.

For reduction of the CQ of RuBpy, we used the method of encapsulation of dye molecules into silicon dioxide nanoparticles [4]. The used technique is based on the Stober's reaction [5].

We prepared several solution of RuBpy dye of various concentrations in isopropyl alcohol, from diluted to saturated one. Stober's reaction in the prepared solutions has occurred. Fluorescence and excitation spectra of the solutions were taken before and after the reaction. It was found that the optimal dye concentration at which the fluorescence intensity reaches a peak and the CQ effect is minimal is 7.83×10^{-11} mol/l.

After obtaining of excitation spectra of the RuBpy solutions with concentration more than $5{,}91\times10^{-11}$ mol/l, CQ of the dye decreased for excitation at the short-wavelength range, in particular for a wavelength of 285 nm, which is responsible for the transition inside the ligand with high energy [6]. We explain this fact by the obstructed steric conditions for the formation of aggregates due to the dye molecule is surrounded by a silica shell.

References:

[1] J.R. Winkler, H.B. Gray, *Chem. Rev.,* **92**, № 3, 369–379 (1992).
[2] V. Balzani, *Chem. Rev.*, **96**, № 2, 759–834 (1996).
[3] P. V. Kamat, *Chem. Rev.*, **93**, № 1, 267–300 (1993).
[4] J. Zhang, *J. Phys. Chem. B. NIH Public Access*, **110**, № 18, 8986–8991 (2006).
[5] W. Stöber, A.Fink, E. Bohn, *J. Colloid Interface Sci. Academic Press*, **26**, № 1, 62–69 (1968).
[6] K. Kalyanasundaram, *Coord. Chem. Rev.*, **46**, 159–244 (1982).

P22. Silicon nanowires modified by nanocomposites materials based graphene oxide for enhanced photodegradation of organic dye

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Dye pollutants in wastewaters are the principal source environmental aqueous contamination. They are classified as environmentally hazardous because they are toxic and degrade slowly. Among the new oxidation methods or “advanced oxidation processes” (AOP), heterogeneous photocatalysis appears as an emerging destructive technology leading to the total mineralization of many organic pollutants [1].
In the present work, we report on the high efficiency of silicon nanowires decorated with graphene oxide and copper nanoparticles (SiNWs-rGO-NPsCu) nanocomposite for the degradation of azo dye like methylene blue and/ou Rhodamine (B) under UV light irradiation [2].The silicon nanowires were elaborated by Ag-metal assisted chemical etching. Also, the effect of voltage and time on the graphene oxide-copper nanocomposite deposit on the silicon nanowires by electrophoretic deposition (EPD) method was study.
The morphology of SiNWs/rGO/NPCu nanocomposite was accessed by scanning electron microscopy (SEM,JEOL-JSM-7610F). The results show that reduced graphene oxide (rGO) is located on the top of SiNWs (Figure1). The absorption spectra of the azo dye solution in quartz cuvettes with an optical path of 10 mm were recorded using HITACHI U-3900H UV–Vis spectrophotometer. It was found that the rate of degradation strongly depends on the photocatalyst parameters studied.

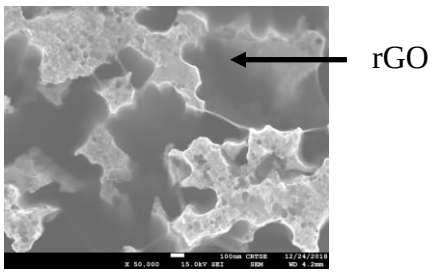

Figure 1: Typical plane view SEM image of the SiNWs/rGO

References

[1] J.M. Herrmann, Water treatment by heterogeneous photocatalysis, in: F. Jansen, R.A. van Santen (Eds.), Environmental Catalysis, Catalytic Science Series, Imperial College Press, chapter 9, London (1999).
[2] S. D. Richardson, C.S. Wilson, K. A. Rusch, Use of rhodamine water tracer in the marshland upwelling system. Ground Water, 42 (5), 678–688 (2004).

P23. Electrochemical contribution to local electromechanical response in P(VDF-TrFe)/$LiNbO_3$

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In this work, we demonstrate an alteration of mechanical, electrophysical, piezo- and ferroelectric properties of P(VDF-TrFE) polymer at the composition of 70/30 mol% in the presence of lithium niobate ($LiNbO_3$) nanofillers. The micro- and nanoscale measurements of the elastic modulus suggest a two-fold increase in the mechanical rigidity of P(VDF-TrFE) film after embedding the $LiNbO_3$ nanofillers. The enhancement of local piezo- and ferroelectric properties of the modified polymer is evidenced by the increase of the direct piezoelectric coefficient from 27.1 pm/V to 36.1 pm/V. This increase has been associated with the significant contribution of the Li-ion stimulus diffusion – the ionic phenomena due to the $LiNbO_3$ nanofillers [1], as unambiguously affirmed by electrochemical strain (ES) response, ES time spectroscopy, and Kelvin probe force microscopy methods.

The results obtained demonstrate crucial achievements towards the polymer nanofillers strategy, $LiNbO_3$ in particular, in attaining the desired functional behavior paving a way towards the development of adavanced sensors, transducers, actuators and piezoelectric devices.

[1] S.Y. Luchkin, K. Romanyuk, M. Ivanov, A.L. Kholkin. "Li transport in fresh and aged $LiMn_2O_4$ cathodes via electrochemical strain microscopy". J. Appl. Phys. 118, 072016, 2015

P24. Facile wet chemical powders synthesis for Copper Oxide thin films preparation and gas sensing applications

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The main objective of this research work is the development and synthesis of nano-architecture structures of copper oxide [1] for obtaining ordered thin films that are, more stable with respect to some specific properties, and can lead to efficient and less expensive gas detection devices [2.3]. In this work, CuO powder, with various morphologies, were successfully synthesized via a simple solution method at low reaction temperature of 60°C. XRD results confirmed the formation of pure single-phase CuO, with a monoclinic structure, in all preparation conditions. Additionally, in all the samples, FTIR spectra show three identical Cu–O vibration modes, which confirms the XRD results. SEM observations show homogeneous and uniform sand-flowers-like CuO nanostructures, which have been successfully synthesized by a simple wet chemical method at a low temperature of 60°C, without the addition of NaOH. The self-assembled three dimensional (3D) nanostructures have average diameters in the range of 4-5 µm. Moreover, the addition of NaOH (1M) leads to a successful production of nano-flake-like CuO nanostructures, with an average size length of about 500 nm. As a result, this reliable low cost method was simple and can be completed in the absence of any surfactant.

Thereafter, by using vacuum thermal evaporation, we deposited the as-prepared copper oxide powder on Si substrate, without any annealing, to obtain p-type copper oxide thin films, for gas sensing applications. SEM/EDS observations and analysis confirm the realization of homogeneous copper oxide thin layer, presenting nano-architectured morphology.

References

[1] G. Jimenez-Cadena, J. Riu, F. Rius, The Royal Society of Chemistry (2007)
[2] D.N. Oosthuizen, D.E. Motaung, H.C. Swart, *Applied Surface Science* (2018).
[3] A. Rydosz, *Coatings*, 8, 425; (2018).

P25. Structural properties of silicone carbide nanoparticles produced by sol-gel method

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The main objective of this work is the synthesis and characterization of silicon carbide nanoparticles.This material is particularly promising for numerous applications in the fields of high frequencies, high temperatures, etc. Silicon carbide exists in many crystalline or polytypes forms. The most studied are the hexagonal polytypes, 4H-SiC and 6H-SiC and the cubic 3C-SiC.In this study, silicon carbide nanopowders (SiC) were synthesized by the sol-gel method, in which sucrose and TEOS were used as precursors of carbon and silicon. After preparation of the soil in the presence of water, solvent (ethanol) and catalysts. The xerogel was stored in an argon atmosphere furnace for carbothermal reduction. other chemical and thermal treatments are carried out on the powder developed to eliminate excess silicon and carbon. The elaborated materials are characterized by FT-IR, Raman, SEM and XRD.The characterization of the samples by the FT-IR technique rvealed the formation of silicon carbide "SiC" through the presence of the absorption peaks at the vibrations of the SiC bond. Raman spectroscopy characterization allowed us to identify SiC polytype. SEM micrographs of SiC powders revealed nanometric particles and the X-ray diffraction patterns of the powders indicated the presence of different SiC phases. The sol-gel method is well recommended for the synthesis of SiC nanopowder provided that the carbothermic reduction is carried out.

References

[1] H. Nosrati, N.Ehsani, .M.Nemati, A.Samariha, J. Sci. Res., 12 (9): 1250-1253, (2012).
[2] R. Ren, Z. Yang, L.L. Shaw, J. Am.Ceram. Soc. 85 (4) 819–827 (2002).
[3] S.Kaci, A. Keffous, and I. Bozetine, ICCESEN Proceeding, Turkey. PP.15–17, (2017).

P26. Ti surface nanoarhitecturing for gliadin identification

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The purpose

Gluten from aliments can be responsible for different diseases [1]. Its electrochemical detection can be made strating from:

- nanostructures have propertis that are desirable for its detection [1]
- electrochemical methods can be used for gluten detection [2]

The main materials and methods used

Nanostructured Ti was the working electrode. Differential pulse voltammetry was used as detection method with an Autolab potentiostat/galvanostat.

The main results obtained

TiO_2 nanotubes were obtained using anodization. Graphene oxide was deposited on top of nanotubes using theree different methods. The method with best results was cyclick voltammetry.

The obtained results for gluten detection with modified Ti electrodes were compared with results obtained with commercialy available Elisa kits.

The main conclusions of the work

Modified Ti alowed gluten detection using electrochemical method.

References

[1] Q. Chen, L. Zhu, J. Chen, T. Jiang, H. Ye, H Ji, S. Tsang, Z. Zhao, T Yia, H. Chen, *Food Chemistry*, **277**, 162–178 (2019).

[2] L. López-López, R. Miranda-Castro, N. de-los-Santos-Álvarez, A. J. Miranda-Ordieres, M. J. Lobo-Castañón, *SENSORS AND ACTUATORS B-CHEMICAL*, 241, 522-527 (2017).

P27. Physicochemistry of Hyaluronic-based Oil Core Nanocapsules for Drug Delivery

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Bioavailability is one of the most important property of newly synthesized drugs. The number of them have low ability to dissolve in water solutions. The work presented herein is focused on preparation the delivery system for not-water soluble compounds. The main idea is based on the hydrophobic modification of the polysaccharide which act as the cover of oil core and stabilizer in one and there is no need for additional low-molecular-weight stabilizers use.

Main materials and methods. Hyaluronic acid, oleic acid (OA), corn oil (CO), dodecylamine, rhodamine B. Tensiometric ring method for intersurface tension observation water-oil phases, DLS for size measurments, Turbiscan for stability in time vs. ionic strength, cytotoxicity assay: neutral red uptake.

Herein, research is focused on nanocapsules as oils delivery systems. The aim of the work was to obtain polysaccharide-based nanocapsules templated on liquid cores by using ultrasound-assisted emulsification. The hydrophobically modified polysaccharide was used to stabilize O/W emulsion by anchoring hydrophobic arms in an oil droplet without the need of using low molecular weight surfactants [1]. Hydrophobic modification concerns influence on lowering the intersurface tension and measurements show that the use of modified polysaccharide is reasonable. Turbiscan measurments let observe the influence of ionic strength. The basic *in vitro* tests show that hydrophobic modification does not influence on cell viability strongly.

To conclude, obtained nanocapsules have great potential as hydrophobic compounds delivery systems and there is more and more known about the physicochemistry of modified polysaccharide and nanostructures.

Acknowledgment

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References

[1] J. Szafraniec, A. Błażejczyk, E. Kuś, M. Janik, G. Zając, J. Wietrzyk, S. Chłopicki, Sz. Zapotoczny. *Nanoscale*, **9**, 18867 (2017).

P28. Nano- and microstructures formed from hydrophobic homopolymer and amphiphilic copolymer – comparative study

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Poly(lactide) (PLA) attracts the attention of researchers due to its biodegradability, biocompatibility and low-priced production process. An exemplary application of PLA is the formation of drug delivery systems (DDSs). The PLA homopolymer or copolymer containing PLA as a hydrophobic block can be used to prepare DDSs.[1]

In the present work, this biopolymer was used to obtain two types of carriers for curcumin, a hydrophobic substance. The first type was formed from poly(2-(methacryloyloxy)ethyl phosphorylcholine)-*block*-poly(lactic acid) (PMPC-*b*-PLA), an amphiphilic copolymer, via the solvent switching method. Other polymeric structures were obtained from a homopolymer using the water/oil emulsion method. As-prepared carriers were characterised using various techniques, such as: optical and confocal microscopy, spectrophotometry and dynamic light scattering. In addition, the experimental results were compared with molecular dynamics simulations (MD). Preliminary studies showed the successful preparation of the nano- and microstructures and effective entrapment of curcumin. The MD simulations enabled the analysis of interaction between the PLA matrix and curcumin at the molecular level. Strong drug-polymer interactions are crucial for effective encapsulation of for hydrophobic compounds inside DDSs.

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

References

[1] Y. Ramot, M. Haim-Zada, A.J. Domb, A. Nyska, *Advanced Drug Delivery Reviews*, **107**, 153-162 (2016)

P29. Interactions of Polycations with Anionic Lipid Membranes

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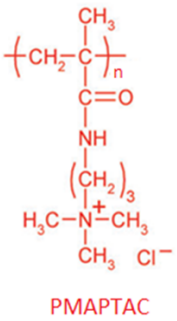
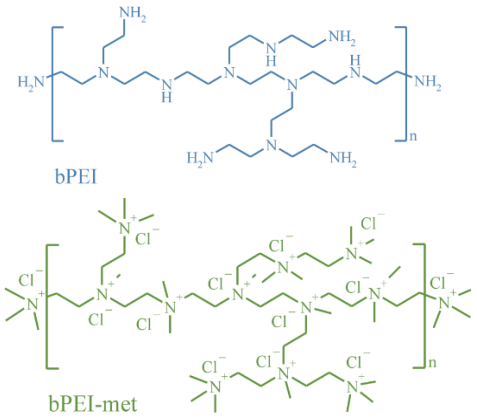
Polycations are an attractive class of macromolecules which are used in many biomedical and biophysical applications, as drug/gene carriers, biocides and coatings for stabilization of liposomes. The chemical structure and concentration of polycation determine its interaction with cellular membranes, and understanding the nature of this interaction is crucial for designing novel nontoxic polycations for these applications.[1]





The aim of our study was to investigate the interaction of various polycations with negatively charged lipid bilayers (POPC/POPS liposomes) representing simple models of cellular membranes. Dynamic light scattering and zeta potential measurements were used to confirm the adsorption of the polymers on the liposome surface and to verify the possibility of vesicle aggregation. The permeability of the lipid membranes treated with polycations was monitored via dye leakage experiments by applying calcein encapsulated in vesicles and fluorescence measurements. Langmuir monolayer measurements were used to study intermolecular interactions between lipid molecules and polycations. In addition, the thermodynamic parameters of these processes were determined using isothermal titration calorimetry (ITC).

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

References

[1] N. Awasthi, W. Kopec, N. Wilkosz, D. Jamróz, J. S. Hub, M. Zatorska, R. Petka, M. Nowakowska, M. Kepczynski, *ACS Biomater. Sci. Eng.*, **5**, 780-794 (2019).

P30. Intercalation of magnetic nanoparticles into bitumen

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Nowadays, the countries all over world use asphalt in order to make roads for vehicles. Road builders use bitumen as “glue” for forming that asphalt which we used to see. Also, the asphalt pavement is subject to frequent destructions by the improper operations of the roads and the abrupt climatic changes of regions [1-2].

But before using this technology in the real life conditions we must know all parameters of the induction heater and which parameters we need in our case [3-4]. The main parameters of the induction heater are the working frequency and the energy consumption [5]. So our laboratory found out the concrete parameters by testing with different frequencies. The needed frequency for the induction heater is 250 kHz at 4 kW consumption. These parameters are chosen relying on the maximum efficiency and economic benefit[6]. All reagents are regarding cheap and the synthesizing technique is easy. Such vehicle works by gasoline generator and “heals” the asphalt pavement.

References

[1] N.A. Gornayev, V.E. Nikishin, A.V. Kochetkov, “Cold apshalt” SNTU Vestnik, 63, 1-15, (2007)
[2] C.P. Bean, J.D. Livingston,“Superparamagnetism”, J. Appl. Phys., 30, 120, (1959).
[3] E.JEOFFROY, M. PARTL, A. Studart, US2018087224, (2015).
[4] A.M. Baranov, “magnetic nanoparticles”, Chem. Journalnaya, 50, 10-40 (2009).
[5] T. Hyeon, “Chemical Synthesis of Magnetic Nanoparticles”, Chem. Commun., 927-934, (2003)
[6] V.V. Trocenko, P.I. Podolyan., “The induction heater”, ESTJ Omsk, 36, 15-28, (2018).

P31. Influence of ions-releasing surfaces on grafting of polymer brushes

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Polymer chains, which are densely packed, stretched, and attached with one end to a substrate, are called polymer brushes. These structures are very promising in many applications such as: controlled drug delivery systems, platforms for controlled cell growth or chemo and biosensors. Furthermore, the new class of conjugated polymer brushes are expected to be used in nanoelectronics. The study of the factors that influence brush growth are of great importance towards formation of well-defined polymer layers with desired thicknesses.

The purpose of our study was to investigate the influence of the surface type on polymer brushes growth. Model brushes (PMMA) were grafted using surface-initiated atom transfer radical polymerization (SI-ATRP) from various flat surfaces. Polymerizations were conducted under the same conditions on indium-tin oxide (ITO), glass and silicon oxide and in the presence of sacrificial initiator. The obtained materials were characterized using atomic force microscopy (AFM), grazing angle FTIR spectroscopy and gel permeation chromatography (GPC).

PMMA brushes were found to grow much thicker on ITO in respect to the other surfaces, demonstrating huge influence of ITO on SI-ATRP kinetic. It was shown that ITO strongly increase the propagation rate of the grafted radicals due to desorption of indium and tin ions which may undergo redox reaction with copper catalyst. The calculated molecular weights of the grafted PMMA chains were greater than the number average molecular weights of free polymers generated in solution, indicating huge differences in the rates of SI-ATRP and ATRP in solution.

Acknowledgements:
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References

[1] A. Gruszkiewicz, M. Słowikowska, G. Grześ, A. Wójcik, J. Rokita, A. Fiocco, M. Wytrwal-Sarna, M. Marzec, B. Trzebicka, M. Kopeć, K. Wolski, S. Zapotoczny, European Polymer Journal, 817-821 (2019).

P32. Luminescent properties of novel Ce-doped ZnO:SiO_2 nanosized films under the action of bovine myoglobin

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In recent years, studying optical properties of nanostructured ZnO films have received considerable attention. The appearance of a narrow intense luminescence band in nanostructured zinc oxide materials over the UV-spectral region determines their application in biosensorics [1, 2]. Namely, introducing dopants into ZnO films allows to achieve increased sensitivity of a biosensor element [2].

In present work, the spectral-luminescent properties of ZnO:SiO_2 thin films obtained by the sol-gel method and doped with Ce^{3+} ions (0.1; 0.3 and 0.5% wt.) were studied. According to the experimental data, modificated films representes high ZnO:SiO_2 luminescence intensity (up to 50–60%) compared to pure zinc oxide samples. In addition, a slight shift in the maximum of the ultraviolet luminescence band (λ_{em} = 358-360 nm) was established after doping by Ce^{3+} ions. It is also interesting to note that ignition of ultraviolet luminescence at 23, 24, 38% was observed during adsorption of myoglobin bovine from solutions of 10^{-8}, 10^{-10}, 10^{-12} M respectively on the surface of ZnO:SiO_2 films with 0.5 mass% of Ce^{3+}.

In conclusion, the synthesized ZnO:SiO_2 nanostructures with Ce- impegration can be used as an effective element in terms of creation optical sensors and improving their properties.

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References

[1] I.A. Nagovitsyn, G.K. Chudinova, A.V. Lobanov, E.A. Borulev, V.A. Moshnikov, S.S. Nalimov, I.E. Kononov, *Chemical Physics*, vol. 37, no. 8, p. 29-35A (2018).

[2] I. Hayrullina, L. Butusov, A. Shulga, I. Nagovitsyn, G. Chudinova, V. Kurilkin, M. Kochneva, *NANOCON 2017, 9th International Conference on Nanomaterials - Research & Application, Conference Proceedings*, p. 161-164 (2018).

P33. A green Functionalization of Poly(ethylene glycol) for Use as biomaterials

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In the present work we have explored a new method to synthesise PEGDM with various molecular weight of PEG (1000, 3000, 6000 and 8000 g/mol). This technique consists on using Maghnite-H^+ as eco-catalyst to replace Triethylamine which is toxic. Maghnite-H^+ is a proton exchanged montmorillonite clay which is prepared through a simple exchange process.[1] Synthesis experiments are performed in solution using Dichloromethane as solvent in the presence of Methacrylic Anhydride. Effect of reaction time, temperature, amount of catalyst and amount of Methacrylic Anhydride is studied, in order to find the optimal reaction conditions. The Synthesis in solution leads to the best yield (98%) at room temperature for a reaction time of 5h. The structure of the obtained macromonomers (PEGDM) is confirmed by FT-IR and ^{1}H-NMR and ^{13}C-NMR, where the Methacrylate end groups are clearly visible. Thermogravimetric analysis (TGA) is used to study the thermal stability of these obtained macromonomers. The presence of unsaturated end group was confirmed by UV-Visible analysis.

Further work is under investigation to use these macromonomers for the synthesis of hydrogels.

References

[1] Belbachir M., Bensaoula A.: Pat. US 7, 094, 823 B2, 2006.

P34. Synthesis and characterization of TEOS/VES silicone nanoparticles

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Silicone nanoparticles are round shaped structures consisted of organosilica materials containing silicon-oxygen backbone and organic side groups. Their structure and properties might be useful in fields of catalysis, nanotechnology and drug delivery [1].

In this study, vinyl-functionalized nanoparticles were synthesized by the co-condensation of Tetraethoxysilane (TEOS) and Vinyltriethoxysilane (VES) using two different methods: the Stober synthesis [2] and the Ouzo effect [3]. The size and shape of the particles were determined using dynamic light scattering (DLS), scanning electron microscopy (SEM) and atomic force microscopy (AFM). The presence of vinyl groups in the structure of the particles was confirmed by ATR IR spectroscopy. The nanoparticles were also cut into very thin slices on the microtome, which allowed us to investigate the inside of the particles. The cross sections were examined by transmission electron microscopy (TEM) and AFM.

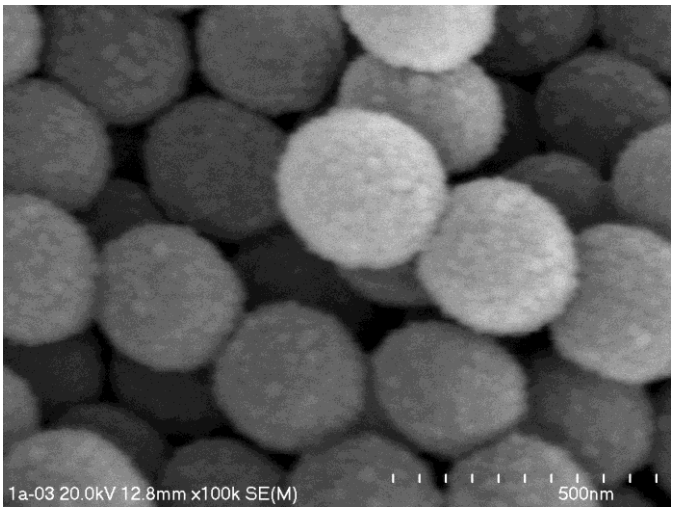

Figure 1 SEM image of particles obtained from TEOS/VES 4:1 mixture

References

[1] J. Wang, Y. Lu, *Mater. Des.*, **111**, 206-212 (2016).
[2] W. Stober, A. Fink, E. Bohn, *J. Colloid Interface Sci.*, **26**, 62-69 (1968).
[3] F. Ganachaud, J. L. Katz, *Chem. Phys. Chem.*, **6**, 209-216 (2005).

P35. Structural Study of Silicon nitride thins films doped with Cerium

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In this work, the structural properties of silicon rich silicon nitride (SiN) thins films doped with cerium (Ce) were studied. The silicon nitride films were prepared with low pressure chemical vapor deposition technique using NH3/SiH4 mixture. Ce films were obtained by evaporation of Cerium oxide (CeO_2) on SiN layers and subsequently annealed within the temperature range of 800-1000°C in N2 ambient.

Structural investigations were performed by Raman spectrometry experiments and scanning electron microscopy. Energy-dispersive X-ray spectroscopy (EDX) characterization results confirm the successful insertion of Ce^{3+} in the silicon nitride at 1000°C annealing for 1 hour.

The results presented in this study indicate that Silicon rich Silicon nitride doped with cerium is a promising material candidate to the development of a silicon-based light source, particularly for visible light emitting applications and photovoltaic solar cells.

P36. Porous silicon double membranes for lithium- ion batteries

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The increasing demands for energy storage sources with a high energy density has been growing rapidly mainly for applications in different domains such as the portable computing and telecommunication and transports. Lithium ion batteries are widely used in mobile electronics and are considered to be one of the best choices as a power source for electric vehicles because of their high energy density. Silicon is one of the most studied for the next-generation anode material for Li-ion batteries due to its high specific capacity 4200mAh/g as anode of lithium-ion batteries compared with the widely-used graphite .However, lithium-ion insertion/extraction process will result in a large volume expansion (320%) of silicon anode, resulting in electrode particle, isolation, disruption of electronic pathways, agglomeration of active particles, capacity loss, etc, and thus very limited cycle life . Nano-structured silicon can play a crucial role in solving these problems. Indeed, porous silicon (PSi) possesses excellent properties for Li insertion, such as efficient electron transport along the axis and large Li ion flux due to the high surface area to volume ratio (200-600 m^2/cm^3).

In this work, Porous silicon (PSi) membranes for lithium-ion batteries (LIBs) anode applications were developed, demonstrated and characterized systematically. Electrochemical measurements were conducted on freestanding porous Si double membranes (10 um+40um). It has been shown that the specific capacity of LIBs was increased remarkably by PSi based anodes. An interesting and encouraging result was obtained. A specific capacity of about 1100-1300 mAh/g was measured .The open circuit potential of the Lithium ion cell with porous Si as anode was about 2.5-3 V vs. Li/Li+ in the open-circuit state.

P37. MODIFICATIONS ON THE CRYSTALLINE STRAIN AND SIZE IN THE PHASE FORMATION OF MULTIFERROIC BISMUTH FERRITE NANOPARTICLES

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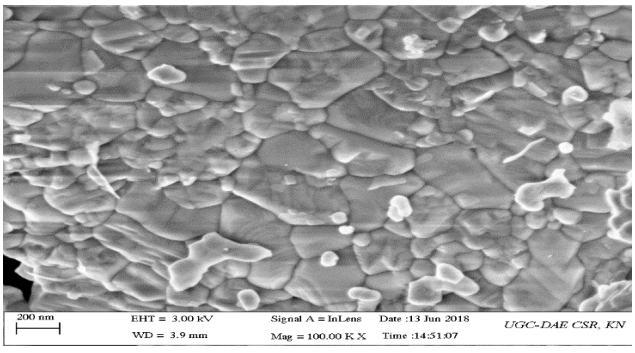
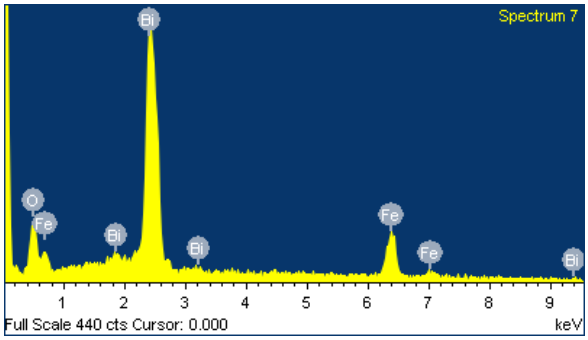
The present work aimed to investigate the effect of micro-strain and crystallite size on multiferroic properties of bismuth ferrite ($BiFeO_3$) (BFO) nanoceramic powders prepared from sol-gel process. The synthesized samples were then calcined in the temperature regime 400-750^{0}C with an interval of 50^{0}C for 1 hour. X-ray diffraction and EDX spectra confirm the single phase of BFO. Crystalline strain of the powder sample has been estimated from W-H analysis. SEM image of BFO tells the fact that morphology of the grown powders is fairly spherical. The other interesting results would be explained in the paper presentation.





References

1.M. Sharmila et. al, Material Science in Semiconductor Processing 34, 109 – 113 (2015)
2.Vijay Kumar et. al, App.Surface.Sci.386, 78 -83 (2016)
3.Prachi Sharma et. al, Journal of Magnetism and Magnetic Materials 374, 18 -21(2015)

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P38. Swift Heavy Ion Irradiation effect on Ferroelectric Triglycine Sulphate (TGS) Single Crystals

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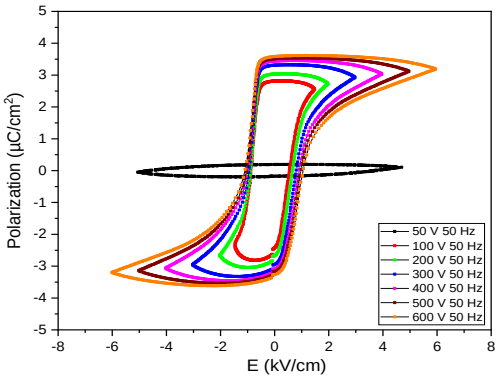
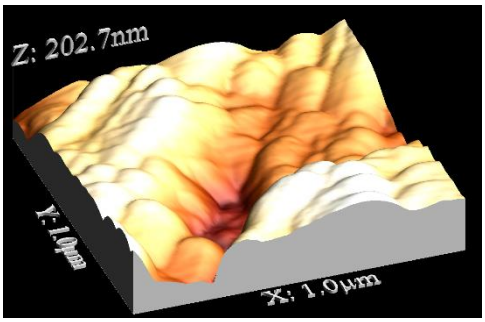
A study on the effect of swift Heavy Ions Ti^{+} (100 MeV) irradiated on TGS single crystals has been performed at various ion fluencies. The optical absorption properties [1-3] of irradiated crystals suggest the fact that due to the creation of defect density, defects band transitions occur nearby to the band edge of TGS. Consequently, optical band gap (Eg) gets modified. Reasonable changes observed in the areas of P-E loops and dielectric constant values reveal that the irradiation induced surface modification greatly affects the electrical and ferroelectric properties of the single crystals upon irradiation. Domain structure changes could also have been witnessed from AFM measurements. The overall results obtained have been correlated with proper scientific interpretation.





References

[1] K.balasubramanian and P.selvarajan,Research in science and technology,2 3,(2010).
[2] S.JStanley, chemical engineering science 61(23) 7850 2006.
[3] P.KBajpai,D.Shah,R.Kumar, Nuclear instrument & method in physics research 244(2006).

P39. Two spectral infrared detectors based on HgCdTe epitaxial layers

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Fabrication and investigation of multielement infrared (IR) detectors for two spectral ranges – mid-wave infrared (MWIR 3-5 μm) and long-wave infrared (LWIR 8-12 μm) on the base of narrow-gap semiconductor thin layers HgCdTe (MCT*)* is reported.

HgCdTe has been used widely over the past 50 years in many detection devices. The band-gap of MCT can be tuned and adjusted to the required spectral region of a particular application by varying the ratio of HgTe to CdTe. MCT technologies are well developed, and narrow-gap semiconductor HgCdTe is one of the basic semiconductors for photon detectors from near IR (wavelength λ~1.5 μm) to long IR (λ~20 μm) and is used in large scale arrays with silicon CMOS readouts.

The topology and technology of two spectral multielement detectors based on epitaxial layers $Hg_{1-x}Cd_xTe$ for the spectral ranges of 3-5 μm (x ≈ 0.3) and 8-12 μm (x ≈ 0.2) has been developed. For IR photodiodes fabrication, HgCdTe layers were grown by the liquid phase epitaxy method on CdZnTe substrates. The thicknesses of MCT layers varied within the limits of 15÷20 μm. Planar HgCdTe photodiodes were formed by B^+ ion doping into epitaxial layers of MCT. The process of photodiodes fabrication included the next technological operations: preliminary chemical preparation of MCT surface; formation of CdTe passivation layers; multilayered photolithography processes; metallization through lift-off photolithography or etching methods to create planar contacts.

The current – voltage characteristics and dynamic resistance of MWIR (3-5 μm) and LWIR (8-12 μm) HgCdTe photodiodes were investigated. Value of parameter R_0A_d for MWIR photodiodes $R_0A_d \approx (0.57 \div 1.08)\cdot 10^5\ \Omega\cdot cm^2$, for LWIR photodiodes $\sim(2\div3)\cdot 10^2\ \Omega\cdot cm^2$, that prove their operability in BLIP mode. Here R_0 is the dynamical resistance of diodes without bias, A_0 is the photodiodes sensitive area.

P40. The synthesis and characterization of a new class of conductive polymers

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

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

P41. Esterification of polyvinyl alcohol with abietic acid in the presence of a green Maghnite-H^+ ctalyzer

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Abietic acid (ABA) a biodegradable compound [1] which is a new research trend derived from pine wood [2] has been conjugated with a number of hydroxyl group of polyvinyl alcohol (PVA) a non-toxic and biodegradable polymer [3], through an esterification reaction in the presence of a green and recyclable catalyst (amontmorillonite sheet silicate clay, exchanged with protons to produce "Maghnite-H^+") [4] The product of the esterification, is obtained with a yield of 87% and a better grafting rate of 45% calculated for a weight ratio of (1: 5); (PVA: ABA).

The successful grafting of ABA on PVA was verified by Nuclear Magnetic Resonance Spectroscopy**^{1}H NMR**, DOSY **NMR** and Infrared Spectroscopy (**FT-IR**).

The catalyst was characterized by **FTIR** and X-ray diffraction (**XRD**).

References

[1] R. CÔTE, and C. OTIS, *REVUE DES SCIENCES DE L'EAU*, **2**,313-324(1989).
[2] M. Ghanmi , B. Satrani , A. Aafi , M. Rchid Ismail , A. Farah and A. Chaouch, *Acta Bot. Gallica*,**156 (3)**, 427-435, 2009
[3] Y. Zhang, B. Pang, S. Yang, W.Fang, S.Yang, T. Q. Yuan, and R.C. Sun, *J. Mater*. **11**,89(2018).
[4] M. Belbachir, and A. Bensaoula, US Patent No. 527 B1 (2001).

P42. Synthesis of 1D and 2D ZnO/Ag/CdS nanocomposites to photon driven hydrogen production

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Hierarchically assembled photocatalysts based on nanoscale semiconductor materials can significantly increase the efficiency of photoelectrochemical processes of water decomposition. This paper demonstrates simple techniques for assembling photoelectrodes of an electrochemical cell based on nanolayers of wide-band and narrow-band semiconductors, such as ZnO/CdS and lowdimensional plasmonic silver particles in a hierarchical manner. The method of synthesizing ZnO nanorods, nanosheets and nanotubes, Ag nanoparticles and CdS thin films is based on the sequential exploitation of electrochemical, hydrothermal and layer-by-layer techniques. Dependence of photoanodes efficiency by using photons for water splitting reaction on its surface morphology based off of hierarchically assembled nanosheets, nanorods, and ZnO/CdS nanotubes was studied. It is shown that electrical resistance in the interface region of photoelectrode - electrolyte on a tubular array of is 1.5 times less in comparison with nanorods and nanosheets. Interlayer deposition of silver nanoparticles into the ZnO/CdS heterostructure semiconductor makes it possible to obtain a ZnO/Ag/CdS nanocomposite with high photocorrosive resistance. Investigation of ZnO/CdS, ZnO/Ag, ZnO/Ag/CdS thin films was carried out by using scanning electron microscopy, X-ray diffractometric, luminescence spectroscopy, UV/visible spectroscopy, impedance spectroscopy, potentiostatic and current-voltage measurements.

P43. Growth and spectral characteristics of $KY(WO_4)_2 : Ho^{3+}$ single crystals

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In the present study we report on growth and spectral characteristics of single crystal layers of potassium yttrium tungstate co-doped with optically inert ions of gadolinium and ytterbium as well as optically active holmium ions to be used as active element of waveguide lasers under direct in-band pumping.

Growth of single crystal layers of KYW were fabricated by liquid-phase epitaxy onto undoped substrate $KY(WO_4)_2$ from a solution of Ho(5at%):$KGd_{0.028}Yb_{0.047}Y_{0.875}(WO_4)_2$ in melted $K_2W_2O_7$; a viscosity of the solution-melt was decreased via adjusting of a concentration of K_2O. The growth was performed in 10-12 wt.% excess of K_2O, thickness of the film was about 140 um, concentration of Ho^{3+} ions ~5.0 at.%.

Based on the XRD data the *b* - parameter equals to 10.341 Å wherein its discrepancy with *b*-parameter of the substrate is about 0.009%. The mention value is about one order of magnitude larger as compared to the limit associated with crack-free growth process [1]. Absorption spectrum of the sample was measured using Fourier spectrometer Vertex 70 (Bruker) with a light polarized along optical indicatrix N_m and N_g (Fig.1). The absorption spectrum is characterized by significant anisotropy for the light having different polarization and it equals to the spectrum of bulk crystal [2]

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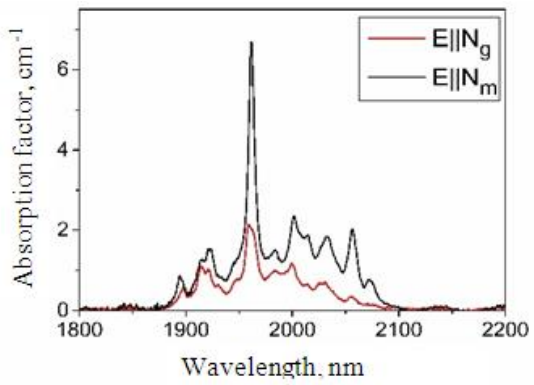

Fig.1. Absorption spectrum of Ho(5at%):$KGd_{0.028}Yb_{0.047}Y_{0.875}(WO_4)_2$

Based on the obtained results we consider the samples under study can be perspective materials to produce active medium for planar waveguide lasers emitting around 2μm.

References

[1] S. Aravazhi, *Appl. Phys. B*, **111**, 433-446 (2013).
[2] V. Lambunathan, *J. Lumin.,* **179**, 50-58 (2016).

P44. Structural Properties of Sol-Gel $BiFeO_3$- Films

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The main purpose is to synthesize $BiFeO_3$ thin films by sol-gel method, i.e. characterization of sample structure on their composition and annealing temperature. The initials for the sol-gel synthesis were salts of metals; ethylene glycol; zitric acid; ethylenediamine. Then the samples $BiFeO_3$ sol-gel materials were annealed at the different temperatures for 20 minutes. X-ray thin-film measurement technique was used to determine the structure.

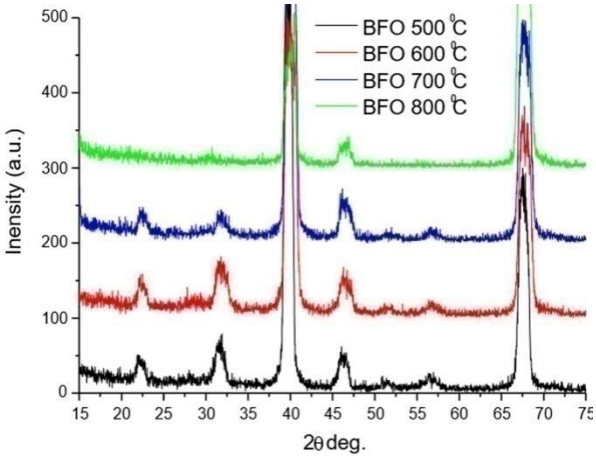

Figure 1- XRD of $BiFeO_3$ sol-gel films

XRD data for $BiFeO_3$ samples annealed at different temperatures were analyzed. It was established that $BiFeO_3$ samples have the different behavior compared to powders [1]. The formation of required with high content phase begins at the temperature of 500 ° C.

This work was funding from the European Union's Horizon 2020 research and innovation programme under Marie Sklodowska-Curie grant agreement No 778070.

References

[1]S. Khakhomov, V. Gaishun, D. Kovalenko, A. Semchenko et. al., *Recent Advances in Technology Research and Education: Proceedings of the 17th International Conference on Global Research and Education Inter-Academia–2018*, **53,** 43-48 (2018)

P45. Investigation of $Bi_{0,9}La_{0,1}FeO_3$ Sol-Gel films by XRD

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$Bi_{0,9}La_{0,1}FeO_3$ thin films by sol-gel method were synthesized and their properties on dependence of the temperature of heat treatment were investigated. Salts of metals, ethylene glycol, zitric acid, ethylenediamine were used for the films synthesis. $Bi_{0,9}La_{0,1}FeO_3$ thin films were annealed at the different temperatures for 20 minutes. XRD was by sliding method measured.

As in the case of $BiFeO_3$ powders [1] and films, perovskite phase formation begins at the temperature of 500 °C. The increasing of the synthesis temperature leads to the decrease of the content of the required phase due to the weak bond of bismuth ions in the crystalline cell.

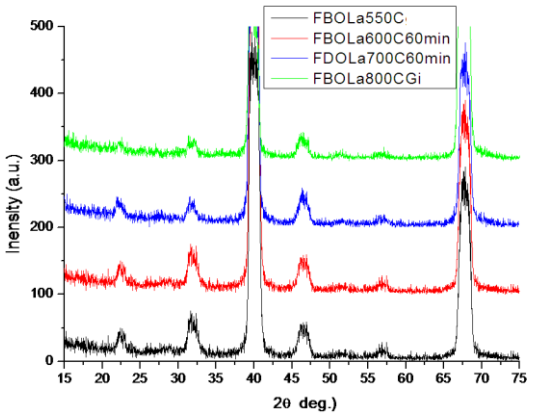

Figure 1- XRD of $Bi_{0,9}La_{0,1}FeO_3$ sol-gel films

This work was funding from the EU Horizon 2020 research and innovation programme under Marie Sklodowska-Curie grant agreement No 778070.

References

[1] S. Khakhomov, V. Gaishun, D. Kovalenko, A. Semchenko et. al., *Recent Advances in Technology Research and Education: Proceedings of the 17th International Conference on Global Research and Education Inter-Academia–2018*, **53,** 43-48 (2018).

P46. Synthesis of $BiFeO_3$ and $Bi_{0,9}Sm_{0,1}FeO_3$ films by Sol-Gel method

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$BiFeO_3$ and $Bi_{0,9}Sm_{0,1}FeO_3$ thin films by sol-gel method were synthesized and the influence of features of sol-gel method and the heat treatment were investigated. Salts of metals, ethylene glycol, zitric acid, ethylenediamine were used for the films synthesis. XRD of $BiFeO_3$ and $Bi_{0,9}Sm_{0,1}FeO_3$ thin films prepared by sol-gel method were analyzed by PDF cards Nr. 01-080-3412 and Nr. 01-078-6349.

As can be seen from the XRD data, the BFO and BFSO reaction products are not monophasic. The doping by samarium leads to the decrease in the content of the perovskite phase due to disruption of the perovskite-type lattice structure by the samarium ion, which is much larger than the other ions that form the crystal lattice.

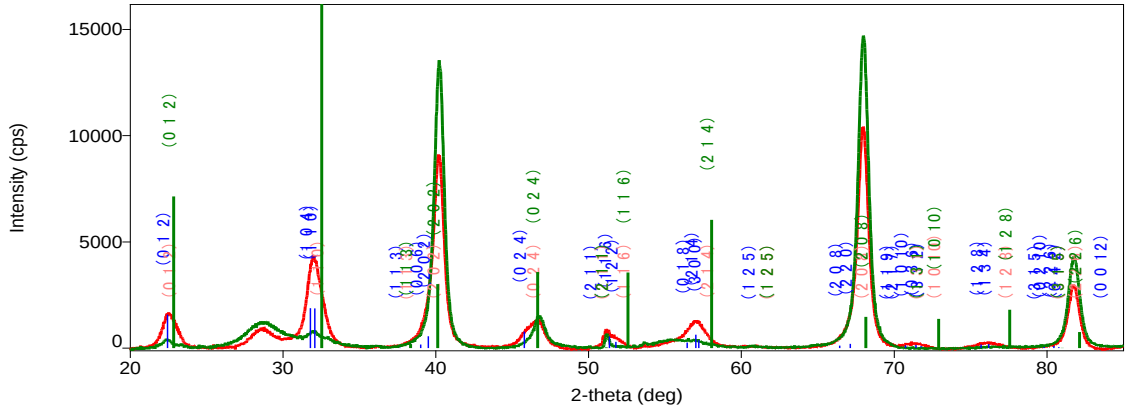

Figure 1 - XRD of $BiFeO_3$(green) and $Bi_{0,9}Sm_{0,1}FeO_3$(red) thin films prepared by sol-gel method

This work was funding from the EU Horizon 2020 research and innovation programme under Marie Sklodowska-Curie grant agreement No 778070.

P47. Modification of interface-controlled parameters of magnetic tunnel junctions by ion irradiation

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Ion irradiation has been used to modify the magnetic anisotropy in magnetic tunnel junction (MTJ) stacks [1,2]. However, the full extent of effects produced by the irradiation on the interface-dependent parameters of MTJs has not been addressed. Here, we irradiated an MTJ multilayer with Ar^+ ions at fluences (Φ) up to $5\times10^{15}\ cm^{-2}$.

The stack was comprised of IrMn/PL/Ru/RL/MgO/FL/Ta/Ru layers, where PL, RL and FL are the pinned, reference and free layers made of CoFe(B) alloys. The effective anisotropy field of the FL, H_{K1}, encompassing interfacial perpendicular (k_{s1}/t), shape ($4\pi M_S^2$), and volume (K_V) anisotropies was measured by ferromagnetic resonance (FMR). Before irradiation $\mu_0 H_{K1} = -10.7\ kG$ (magnetization in plane) and the tunnel magnetoresistance (TMR) was of 193%.

The magnitude of the anisotropy field decreased with increasing fluence (fig. a, c) following the lowering of M_S caused by intermixing at the FL/Ta interface. The TMR dropped to 74% at $\Phi = 3\times10^{13}\ cm^{-2}$, following the decrease in R_{AP} (fig. b), resulting from the creation of defects within the MgO barrier, acting as spin-independent tunnelling channels shunting the spin-dependent one. Above $\Phi = 10^{14}\ cm^{-2}$, the RL became decoupled from the PL as seen by the two loops in R(H) (fig. b) and the appearance of an additional FMR line (fig. c).

Other effects of the irradiation, particularly those concerning the magnetic damping, will also be discussed.

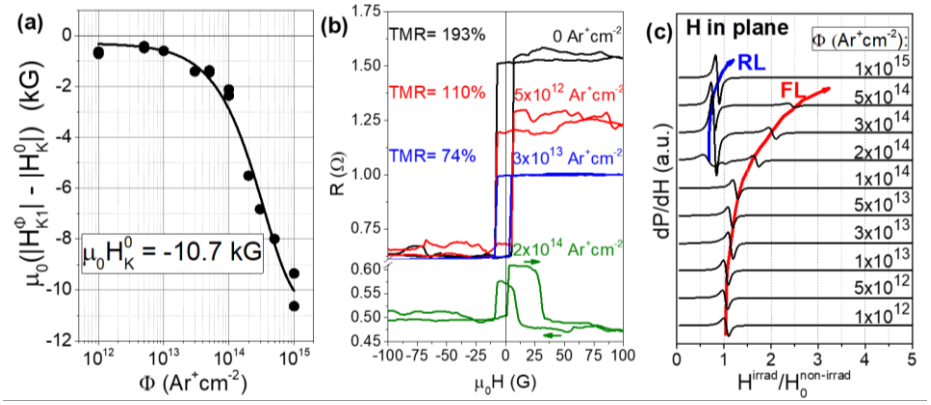

Figure. (a) changes in magnitude of the anisotropy field versus ion fluence; (b) R(H) loops for selected ion fluences; (c) FMR spectra for increasing ion fluences (H-axis normalized by resonance field before irradiation).

References

[1] B.M.S. Teixeira et al. Appl. Phys. Lett. **112**, 202403 (2018);
[2] T. Devolder et al. J. Appl. Phys. **113**, 3 (2013);

P48. Conjugation of nanomaterials in cellulose filter paper for superior water filtration

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The quality of water resources is deteriorating regularly and the demand for potable water at affordable cost has been increasing along with industrialization and population growth. Globally, unsafe and contaminated water supplies pose significant risks to human health and the environment. Recent advancements in material technology has helped the scientific community to develop economic technological solutions to existing problems. The aquatic environment should be free from chemical and biological contamination. The interfacing of nanomaterials with conventional water process engineering can offer new opportunities in water management. The present work deals with synthesis of different metal oxide nanomaterials and their conjugation with cellulose foam filter paper. CuO, ZnO, and Ag_2O nanomaterials were synthesized using economic chemical methods and further impregnated in cellulose filter paper. The listed nanomaterials were selected based on their potential antimicrobial activity against a broad range of microbes. Different microscopic and spectroscopic techniques such as DLS, UV-Vis, FTIR, FESEM, XRD, TGA, zeta potential etc. were used to confirm the formation of nanomaterials and further their impregnation inside filter paper. The nanomaterial impregnated filter paper was evaluated for its antimicrobial properties against different microbial strains. The nanoengineered filter paper demonstrated superior filtration performance compared to unmodified/pure filter paper. The variation in filter paper performance was also observed with size and nature of nanomaterials.

References

[1] S. Jain, G. Bhanjaja, S. Heydarifard, N. Dilbaghi, M.M. Nazhad, V. Kumar, K.H. Kim, and S. Kumar, *Carbohydrate Polymers*, **202**, 219-226 (2018).

[2] S. Heydarifard, K Taneja, G. Bhanjaja, N. Dilbaghi, M.M. Nazhad, K.H. Kim, and S. Kumar, *Carbohydrate Polymers*, **181**, 1086-1092 (2018).

P49. Polarization and Piezoelectric properties of ZnO nanoparticles/nanorods interacting with various dopant and PVDF structures: molecular modeling and experiments

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Zinc oxide (ZnO) is a versatile material, which has unique optical, semiconducting and most important piezoelectric properties [1]. Alternatively, poly(vinylidene fluoride) (PVDF) and PVDF-trifluoroethylene (TrFE) (i.e., its copolymer) are piezoelectric polymers, has been used for dynamic strain sensing and energy harvesting [2]. Ideally, piezoelectric materials should possess high piezoelectricity, while remaining conformable and flexible like piezo-polymers. One of the method for simultaneously achieving improved piezoelectric and mechanical performance is by embedding piezoelectric ZnO nanomaterials into PVDF polymer matrices for enhancing piezoelectricity of such composite architectures [3]. Similarly is possible to enhance piezoelectric property in ZnO structures by doping it's crystals by various atomic dopants [4].The goal of this study is to perform the estimation of the ZnO crystal cluster models, "ZnO+PVDF" and "ZnO+A" composite structures and properties using molecular modeling and computational physical properties calculations. We taken out the initial unit cell crystal structure of ZnO crystal in the hexagonal P63m group [6-8] from CCDC data base (lattice constant a = 3.249Å and c = 5.204Å) [6] and reconstruct it to the HyperChem [9] workspace, where built first a minimal ZnO cluster (from 18 atoms) and second a nanorod ZnO model cluster (from 72 atoms). Then we construct here the "ZnO+PVDF" and "ZnO+A" models with various atoms. Computational molecular models of ZnO cluter, PVDF chain and composite of "ZnO+PVDF" were considered and performed in this study using HyperChem software by various semi-empirical methdos PM3, MNDO/d in restricted/unrestricted Hartree-Fock (RHF/UHF) approximation [9, 10]. For "ZnO+A" the a*b initio* methods was used with various basis set (3-21G with 675-735 primitive Gaussians, and 6-31G* with ~1200 Gaussians) [9], depending of the atom "A". Distance between "A" and cluster's centre of mass ~ 3.5 Å. Initial pure ZnO model were calculated using both approaches. Models are presented on Fig. 1, results in Table 1.

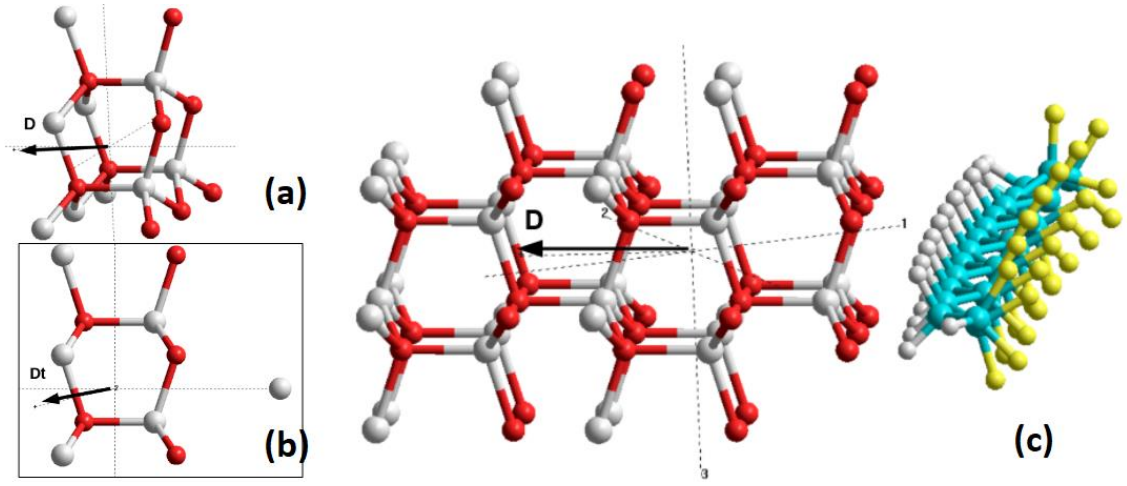

Figure 1. ZnO cluster model: a) ZnO initial minimal cluster, b) ZnO nanoparticle interacting with atom "A", c) ZnO nanorod interacting with PVDF chain in composite structure model.

Table 1. Polarization characteristics of "ZnO+PVDF" composite cluster, obtained by various methods.

Model	Parameters	Methods (in RHF/UHF)						Other data		
		PM3	AM1	MINDO/d	ZINDO/S	Ab initio 3-21G	Ab initio 6-31G*	Calc. P, C/m^2 [7,8]	Experimental [1, 5]	
									P, C/m^2	d*, pm/V
ZnO-18	Dipole, Debye	17.728		15.123		16.1815	18.975			
	Polarization, C/m^2	0.1032		0.0885		0.0947	0.111	0.07-0.08		9.9-12.4
ZnO-72	Dipole, Debye	13.441	19.788	11.739	53.853					
	Polarization, C/m^2	0.0944	0.139	0.0825	0.101			0.07-0.08		9.9-12.4
ZnO-18 + Cr	Dipole, Debye					11.8837				
	Polarization, C/m^2					0.0669			0.062	120
ZnO-18 + V	Dipole, Debye					4.627				
	Polarization, C/m^2					0.0258			0.02	110
ZnO-18 + Mg	Dipole, Debye					15.245				
	Polarization, C/m^2					0.08535			0.002	54
ZnO-18 + Y	Dipole, Debye					6.0831				
	Polarization, C/m^2					0.0339				420
PVDF12	Dipole, Debye	25.12	24.343	29.971	34.429					
	Polarization, C/m^2	0.167	0.162	0.199	0.07			0.1	0.1	20-40
PVDF12+ ZnO-72	Dipole/dist., Debye/Å	45.082/10.0 45.338/10.5	47.38/10.0 50.89/11.5	51.927/10.0 47.844/11.5	95.872 90.50					
	Polarization, C/m^2	0.154 0.155	0.162 0.174	0.1775 0.1634	0.0992 0.0903					

Data obtained show good agreements with experimental data. However, it is only first step of our calculations and work will be continued further, similarly as in our previous calculations of the piezoelectric coefficients in PVDF and Graphene-based polymer ferroelectrics [9-11]. Experimental part supported by AFM/PFM measurements. Authors wish to acknowledge the Russian Foundation for Basic Researches (RFBR) grant # 19-01-00519 A.

References

1. N. Sinha, S, Goel, A.J. Joseph, H. Yadav, K. Batra, M.K. Gupta, B. Kumar, *Ceramics International* **44,** 8582–8590 (2018).
2. V.M. Fridkin, S. Ducharme. *Ferroelectricity at the Nanoscale* (Springer), 30-65 (2014).
3. T. Furukawa, M. Date, E. Fukada, *Journal of Applied Physics* 51, 1135 (1980).
4. J.S. Dodds, F.N. Meyers, K.J. Loh, *IEEE SENSORS JOURNAL* **12 (6)**, 1889-1890 (2012).
5. K. Batra, N. Sinha, S. Goel, H. Yadav, A.J. Joseph, B. Kumar, *Journal of Alloys and Compounds* **767** 1003-1011 (2018).
6. K. Kihara, G. Donnay, *The Canadian Mineralogist* **23** (4), 647-654 (1985).
7. P. Gopal, N.A. Spaldin, *Journal of Electronic Materials* **35 (4),** 538–542 (2006).
8. S.-H. Park, D. Ahn, *Appl. Phys. Lett.* **87**, 253509 (2005).
9. *HyperChem 8.0, Professional Edition*. (Gainesville: Hypercube. Inc.) (2010).
10. V.S. Bystrov, I.K. Bdikin, M.Silibin, *et al.*, *J. Mol. Mod.*, **23,** 128 (2017).
11. V. S. Bystrov, I. K. Bdikin, M. V. Silibin, X. J. Meng, T. Lin, *et al.*, *Ferroelectrics* (2019)

P50. Properties optimization by Al doping of ZnMgO for transparent conductive oxide (TCO) films

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ZnMgO with high natural abundance and low cost is one of the most promising alternatives to the CdS buffer layer in the CIGS and CZTS solar cells [1]. Including this material in a pure sulphide CZTS based solar cell, its numerical simulation carried out by SCAPS-1D software shows a very promising conversion efficiency η of 8.89% compared to the reference structure with conventional CdS buffer layer (η = 9.39 %). In this work, Zn0.9Mg0.1O polycrystalline films were successfully grown by the spin-coating method and Post-annealing in oxygen ambient has significantly improved their properties. In order to obtain good conductivity and high transmittance of the transparent conductive oxide (TCO), we doped it by Al and analyzed their structural, electrical and optical properties. The Al concentration was varied between 0.05 to 0.2%. The XRD patterns show that the all samples exhibit wurtzite crystal structure with (002) preferred orientation. The doping of Ga was calculated and confirmed by EDX. The weighted average transmittance in the visible range exceeds 85% in all films. So, enhanced transmittance and higher optical band gap obtained compared to the pure ZnMgO thin film. Finally, the resistivity of the films decreases gradually with increasing of Ga-content.

Reference

[1] M. Nardone, Y. Patikirige, C. Walkons, S. Bansal, T. M. Friedlmeier, K. E. Kweon, J. B. Varley, V. Lordi, IEEE 45th Photovoltaic Specialists Conference (PVSC) Waikoloa, HI, USA, June 10-15, 2018.

P51. Li vacancies effect onto Li/Si alloys properties: theoretical investigation

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Energy storage is a crucial aspect of integrating renewable energy sources in power grids, which makes the development of efficient high-capacity batteries an important technological field [1]. In this contribution, Li/Si alloys properties have been predicted with DFT investigations. We use pseudopotential approximation to simulate electronics, elastics and optical properties $Si_{1-x}Li_x$ structure.

Table: Fermi Level variation with Li vacancy concentration (V)

	V_1	V_2	V_3	V_4	V_5	V_6	V_7
E_F (eV)	5.03	4.80	4.93	4.73	4.80	4.44	4.33

We study the evolution of Li vacancy on structure and her physical properties. This type of calculation method could be applied as an easy and effective tool for predicting the potential performance of new lithiation/delithiation materials. Potential study directions in this research field and difficulties that the field still faces are discussed at the end.

References

[1] Whittingham M S 2008 *MRS Bull.* **33** 411

P52. Local piezoelectric properties of dipeptide nanotube structures

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In the past 20 years, various types of peptide nanostructures (PNT) have been found: nanotubes, nanoballs, nanorods, nanosheets. Due abnormal 2D- and 3D-shape of these materials demonstrated unique physical properties. It can be used in important applications: sensors, gernerators etc. For effective commertional devise there several parameters: technology systesis problems and cost, bio and ecology acceptability, value used for the practical application of the effect. Recent investigation and molecular modeling of the formation, structure and physical properties of various types of the peptide nanotubes, 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 exibits some specific similar properties. For example, the branched-chain amino acids (BCA) can support ferroelectricity in such structures as liquid crystals and transmembrane ion channels. 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]. 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 [4].

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. Since PFM only provides an effective piezoresponse and average value of surface vibrations caused by the non-uniform distribution of the electric field we compared the results with a well-known piezoelectric, such as $LiNbO_3$ (LNO), PZT. PFM measurements we did in same conditions (cantilever, frequency, AC amplitude, AFM gains, force, speed etc.) and same equipment. Thus, the piezoelectric effect in PNTs piezoresponse coefficients can be very accurate estimate between different type of di-peptaides.

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[1] C. H. Gorbitz, *Chem Eur J.*, **7**, 5153–5159 (2001).
[2] E. Gazit, *FASEB J.*, **16**, 77-83 (2002).
[3] V. S. Bystrov, et al Ferroelectrics, **440**, 3–24 (2012).
[4] H. R. Leuchtag and V. S. Bystrov, *Ferroelectrics*, **220** *(3-4)*, 157-204 (1999).

P53. Development of new materials for air purification applications

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In the recent past, the fabrication of new TiO_2/reduced graphene oxide (rGO) immobilized in poly (vinylidene difluoride-co-trifluoroethylene) (P(VDF-TrFE)) electrospun membranes was reported by our group [1]. It was shown that the synthetic membrane is a promising photocatalyst for degradation of organic pollutants in aqueous systems.

The capability of this membrane for air filtration applications has been furtherly investigated together with the optimization of a photo-degradation lab scale reactor.

This study, targeted oxides of nitrogen (NOx) and volatile organic compounds (VOCs) to evaluate the membrane performance as an air purifier.

These mentioned gases are major pollutants in air, associated with adverse health concerns becoming one of the growing problems that world is facing today. In this regard, our aim is to bring the practical usage of this membrane into the real-world air filtration applications.

References

[1] N. A. F Almeida, et al. J. Mater. Sci. 51 (2016) 6974-6986

P54. TiO_2-rGO nanocomposite immobilized in P(VDF-TrFE): a sunlight active and reusable photo-catalyst for the elimination of metoprolol in water

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An increase of the consumption of metoprolol (MTP) used for the treatment of heart diseases, and the inefficiency of its removal in wastewater treatment plants, raise concern regarding the contamination of aquatic systems [1]. Titanium dioxide (TiO_2) has received increasing attention for removal of organic contaminants from environment. Nevertheless, TiO_2 drawbacks such as large bandgap and surface redox reaction needs to be overcome in order to achieve a high performance in the photocatalytic degradation of pollutants [2]. In this regard, band gap nanoengineering such as doping and/or introducing carbon-based materials to nanoparticles (NPs) of TiO_2 for longer life span of electron-hole pairs are suggested. Here we report the high degradability of MTP in buffered aqueous solution (pH 7), using a TiO_2-rGO (TiO_2-reduced graphene oxide) nanocomposite and TiO_2/rGO - poly(vinylidene difluoride-co-trifluoroethylene) P(VDF-TrFE) membrane previously developed in our group [3] under simulated solar light.

Using the TiO_2/rGO nanocomposite in suspension, 98% of MTP total removal after only 60min was registered, which is much higher than using only the TiO_2 NPs that only originate 52% total removal of MTP after 60 min.

In addition, the immobilization of TiO_2/rGO nanocomposite in a P(VDF-TrFE) membrane prepared by wet phase inversion, not only showed a good photocatalytic performance (around 88% of removal after 180 min irradiation) and also facilitates the catalyst recovery which makes it eco-friendly and reusable. Importantly, the photocatalytic performance of the membrane was maintained after second (94%) and third cycle (87%).

These results indicate the great potential of TiO_2/rGO-P(VDF-TrFE) membrane for the removal of MTP from contaminated waters, and points to further studies using other organic contaminants towards future water purification applications.

References:

[1] J. Maszkowska, S. Stolte, et al., Sci. Total Environ 493 (2014) 1122–1126.
[2] X. Kang, S. et al, Catalysts 9 (2019) 191-223
[3] N. A. F Almeida, et al. J. Mater. Sci. 51 (2016) 6974-6986

P55. Modeling of dichalcogenide MoS_2 monolayers and its composites with PVDF/P(VDF-TrFE)

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Transition metal dichalcogenide MoS_2 monolayers is very promising for many applications, especially in the fields of in optics as emitters and detectors, in electronics a transistors. It is first of all due that they have a direct band gap Eg. Important aspect is also that the value of this band gap Eg could be controlled and changed by some external influences. For example. one of the possible way is to cover the MoS_2 layers by the polymer ferroelectrics layers, such as PVDF/P(VDF-TrFE) and create the composite heterostructure with controlled polarization switching in the ferroelectric layer to induce the optical band gap changes in MoS_2 structure. One of the example of such devices was recently demonstrated by group from National Key laboratory of Infrared Physics of Shanghai Institute of Technical Physics of Chinese Academy of Sciences (by scientific group, including Hong Shen, Xiangjian Meng et al.) [1].

The several results of the molecular modeling of the MoS_2 layers and calculations of its interactions with PVDF chain are presented in this work as a several simple models of such heterostructure (Fig.1).

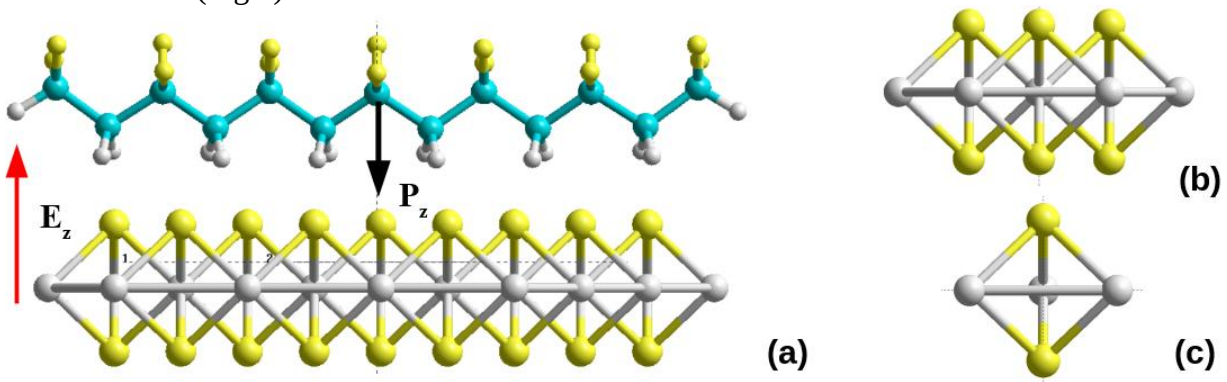

Figure 1. Model of interacting PVDF chain with MoS_2 layer: a) PVDF and MoS_2 layer in Y-projection, b) MoS_2 model from 6S atoms and 7Mo atoms, c) MoS_2 model from 2S and 3Mo atoms.

Using DFT and *ab initio* calculations in 3-21G basis for unrestricted Hartree-Fock (UHF) approximation we calculated the energies E HOMO and E LUMO under various electric field E_z values. In this case the computed changes of the band gap Eg = E LUMO - E HOMO under influence of electric field E_z from polarized PVDF was obtained. In this model PVDF have polarization $P_z \sim 0.167$ C/m^2, creating electric field $E_z = P_z/2\varepsilon\varepsilon_0 \sim (1 – 2)*10^9$ V/m (for MoS_2 dielectric permittivity $\varepsilon \sim 4 – 6$ [2, 3]).

Decreasing of Eg with rising of electric field, computed for 1 layer MoS_2 model in this case, was reached approximately $\Delta Eg \sim 0.08$ eV per $\Delta E_z \sim 1$ V/nm. This result is comparable with data obtained in work [1] (Fig.2) by DFT calculations with PBE functional within DMol^3 code for triple-layer MoS_2 model. In this case of 3-layers structure decreasing of Eg was obtained at the level of $\Delta Eg \sim 0.24$ eV per increasing of electric field on $\Delta E_z \sim 0.8$ V/nm.

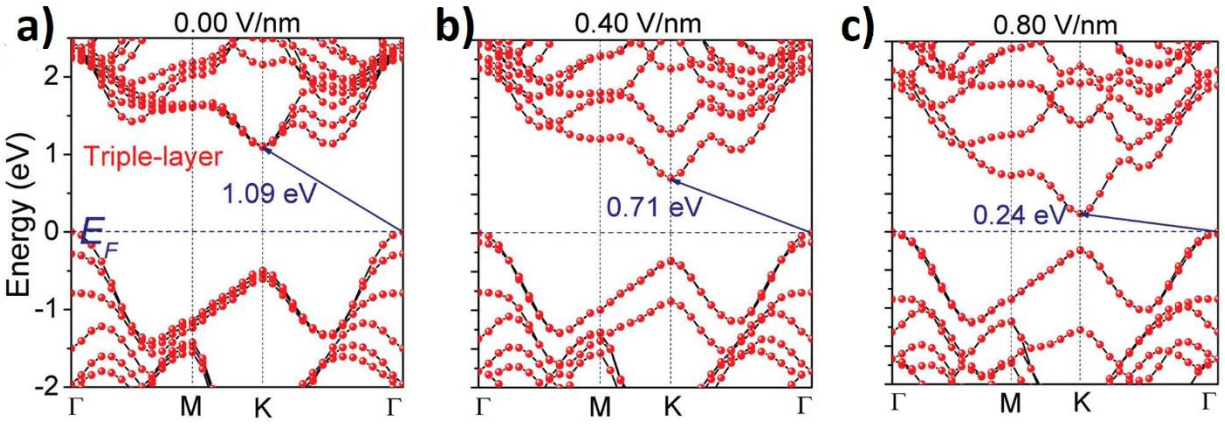

Figure 2. The band structures evolution of triple-layer MoS_2 under different external electric field (0.0, 0.4, and 0.8 V/nm) by first-principles DFT calculations from [1]: a) zero electric field, b) in electric field with $E_z = 0.4$ V/nm, c) in electric field with $E_z = 0.8$ V/nm.

Further study necessary to investigate more details of this interaction of PVDF and P(VDF-TrFE) with various MoS_2 layers using more developed VASP software with novel hybrid functionals similarly as in our works [4, 5]. This work is supported by the Russian Foundation for Basic Researches (RFBR) grant # 19-01-00519 A.

References:

1. Xudong Wang, Peng Wang, Jianlu Wang, *et al. Adv. Mater*. 27, 6575–6581 (2015).
2. E.J.G. Santos, E. Kaxiras. *ACS Nano*. 7 (12), 10741-10746 (2013).
3. X. Yan, L. Zhu, Y. Zhou, Y. E, L. Wang, X. Xu. *Applied Optics*.54 (22), 6732-67-36 (2015).
4. L.A. Avakyan, E.V. Paramonova, José Coutinho, Sven Öberg, V.S. Bystrov and L.A. Bugaev. *J. Chem. Phys.* 148, 154706 (12 pages), (2018).
5. V.S. Bystrov, L.A. Avakyan, E.V. Paramonova, and José Coutinho. *J. Chem. Phys. C.* 123 (8), 4856–4865 (2019).

P56. Mechanical properties and fracture mechanism of Ti_3Al intermetallic produced by powder metallurgy and casting processes

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Due to its low density, good oxidation and creep resistance at high temperatures combined with high strength, Ti_3Al intermetallic is used in aerospace, automobile and other industries [1]. However, the greatest disadvantage is its high brittleness. Room temperature ductility and high temperature properties of Ti_3Al-based alloys have been improved by the addition of the *β* (bcc)-stabilizing elements such as Nb and Mo [2]. The room and high-temperature compression strength and ductility, microstructure and fracture mechanism of Ti_3Al-Nb-Mo intermetallic produced via powder metallurgy (PM) and vacuum melting and casting processes have been investigated. Non-porous PM compacts were obtained via vacuum hot pressing of powders produced by mechanical alloying. Prior to compression tests, all samples were homogenized by a solution treatment at 1050 °C for 1h, followed by water quenching. Subsequent aging at 800 °C during 24 h induces small content of *O*-phase. The compression tests were performed from room temperature to 500 °C in vacuum. Detailed microstructural characterization has been evaluated by scanning electron microscopy (SEM), followed by electron dispersive spectroscopy (EDS) and X-ray diffraction analysis. Fracture topography was examined by SEM. The yield strength of all samples increases with temperature up to 250 °C after which it decreases. Ductility increases through the whole temperature range. The presence of *O* phase contributed to ductility increase in aged alloys, while negligibly lowering yield strength. Registered drop in the yield strength of aged alloys compared with non-aged ones was mostly influenced by precipitation of α''_2 particles. Values of compressive mechanical properties of PM compacts were higher than those of castings. Powder metallurgy processing (PM) demonstrated superior mechanical properties of titanium aluminides to those processed by conventional ingot metallurgy due to microstructural homogeneity, minimized segregation and refined grain size. Mixed fracture modes are operative at all temperatures.

Acknowledgements

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References

[1] F.H. Froes (ed.), *Titanium: Physical Metallurgy, Processing, and Applications*, ASM International, Materials Park, Ohio (2015).

[2] S. Djanarthany, J.C. Viala, and J. Bouix, *Mat. Chem. Phys.*, **72**, 301(2001).

P57. The effect of picosecond laser on silver target – surface modification and nanoparticles production

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The effect of picosecond lasers (pulse duration 40 and 150 ps) on silver target was investigated in gaseous (air) and liquid (water) surrounding. Morphological and chemical surface changes in both media were analyzed, as well as the phenomenon of nanoparticles (NPs) production by laser ablation in liquid (LAL) process. LAL is a subject of extensive research in the last decade, as it is efficient, clean, and can provide surfactant-free, biocompatible NPs with high stability [1]. Due to unique properties, silver nanoparticles can be applied as antimicrobial agents, in bioimaging, chemical (catalyzers), electronic industry (e.g., sensors), etc. Intermediate picosecond pulse length (150 ps) applied here has its advantages in obtaining of nanoparticles [2]. In case of ultrashort (< 10 ps), especially femtosecond pulses, nonlinear effects lower the absorbed energy used for ablation, while in longer, nanosecond domain, the efficiency of the process is diminished by the plasma plume in front of the target ("shielding" effect) as well as melting of the target. In this work, obtaining of nanoparticles was studied in dependence of different process parameters (pulse energy 2-30 mJ, different irradiation times, target position above and below lens focus). Nd:YAG lasers were employed, at the wavelength of 1064 nm and pulse frequency 10 Hz. Characterization of the target surface (e.g. morphology), size distribution of NPs and their mass concentration (in water) were performed using scanning electron microscope (SEM), dynamic light scattering (DLS) technique as well as optical absorption spectroscopy (ultraviolet-visible spectrophotometer), and inductively coupled plasma optical emission spectrometer (ICP-OES), respectively. The optimum results were obtained with the target in front of the lens focus, applying pulse energy of ~10-20 mJ, and the obtained nanoparticles show good characteristics regarding size, yield and stability.

Acknowledgements
This research was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia through project no. 172019.

References

[1] D.L. Andrews, Photonics, Volume 3: Photonics Technology and Instrumentation, Wiley, New Jersey (2015).
[2] J. Stašić, Lj. Živković, M. Trtica, *J. Nanopart. Res.*, 18, 366 (2016).

P58. Comparison of surface topography in machining Ti alloys for biomedical applications: Correlative microscopy approach for qualitative and quantitative analysis

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In the last decades, the demand for biocompatible materials has increased these materials are widely used to manufacture medical devices such as dental and surgical implants. The improvement of these materials used in the manufacture of biocomponents is a constant objective in research focused on reducing negative impacts on patients.

Currently, the most commonly used metal alloy in the biomedical industry is Ti-6Al-4V [1]. Although it has interesting properties, this material may present a risk to the patient due to the presence of vanadium. Alternatively, the Ti-6Al-7Nb alloy may be a candidate to replace traditional alloys, but many studies are still required for the understanding of the fabrication of biomedical component techniques, for example, the machining process.

The study of surface topography, through modern microscopy techniques, presents great potential to optimize the manufacturing processes through the machining of this material. The objective of this work is to propose a correlative microscopy technique [2] developed for the comparative analysis of surfaces machined by the turning process of the Ti-6Al-4V and Ti-6Al-7Nb alloys. This technique was based on the association of the extended field-depth method from Light Microscopy (LM) with Scanning Electron Microscopy (SEM) and microanalysis modes. The correlative microscopy allowed a direct correspondence between the cutting conditions and the properties of these Ti alloys, through the analysis of the machined surface, combining the advantages of SEM and LM.

References

[1] Costa, B.,*et.al.* Vanadium ionic species from degradation of Ti-6Al-4V metallic implants: In vitro cytotoxicity and speciation evaluation. MAT SCI ENG *C*-MATER, 96, 730–739 (2019).

[2] Vicidomini, *et.al.* A novel approach for correlative light electron microscopy analysis. Microsc Res Techniq, 73, 215–224 (2010).

P59. A comparative study between conventional drilling and helical milling in titanium alloys for medical applications

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Hole making in medical devices is a common finishing manufacturing operation. Hence the need to refine and develop methods that allow to make them more efficiently and with the desired quality, so that the function to be performed is not compromised, it is necessary to adjust the manufacturing method.
Compared to conventional drilling, helical milling offers the economic advantage of being able to drill holes of different diameters with the same tool [1]. Some previous studies revealed that the required cutting forces are considerably lower than those of drilling, there is a lower generation of high temperatures and a lower probability of occurrence of adhesion of the material to the tool. This results presents a clear advantages of this milling in terms of tool life and less burr both at the entrance and at the exit of the hole, which removes the need for finishing operation such as reaming or countersinking [2], [3].
The objective of this work is to be able to compare the quality of surfaces in terms of Ra and Rt generated by drilling and helical milling in two titanium alloys in a series of tests with different cutting parameters.

References

[1] O. M. Ozturk, Z. M. Kilic, and Y. Altintas, “Mechanics and dynamics of orbital drilling operations,” *Int. J. Mach. Tools Manuf.*, vol. 129, no. February, pp. 37–47, 2018.

[2] X. Da Qin, X. T. Sun, Q. Wang, S. M. Chen, and H. Li, “Comparative Study on Helical Milling and Drilling of Ti-6Al-4V,” *Key Eng. Mater.*, vol. 499, pp. 200–204, 2012.

[3] S. Sharif, E. Abd, and H. Sasahar, “Machinability of Titanium Alloys in Drilling,” *Titan. Alloy. - Towar. Achiev. Enhanc. Prop. Divers. Appl.*, vol. 3, no. c, 2012.

P60. Sintering Atmosphere Effect on Powder Injection molded AISI-420 stainless steel powder

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This study concerns determination of effect of sintering atmosphere on Powder Injection Molded AISI-420 stainless steel parts. Samples, formed from the feedstock by mixing the prealloyed AISI-420 stainless steel powder with a multi-component binding system, are made subject to sintering at different atmosphere (pure hydrogen and Argon) following the debinding process. Samples that are sintered under such conditions giving way to the highest relative density, are head treated thermal process. Sintered and heat treated samples have been subjected to microstructural analysis and mechanical test. Mechanical tests such as hardness measurement and tensile test as well as microstructural characterization such as X-ray diffraction (XRD), scanning electron microscope (SEM) and elemental analysis all have shown that the thermal process increases strength of the material. However, it is observed that alloy AISI-420 produced by the method of PIM is at such level to compete with the characteristics of cast alloy AISI-420.

References

[1] German, R.M., Bose, A. 1997. Injection Molding of Metals and Ceramics, Metal Powder Industries Federation, Princeton, NJ, 11.
[2] Davis, J.R., Stainless steels, ASM international, 1994
[3] Berrettaa, J.R., Rossib, W., Nevesc, M.D.M., Almeidab, I.A., Junior, N.D.V., Pulsed Nd: YAG laser welding of AISI 304 to AISI 420 stainless steels, Optics and Lasers in Engineering, 45(9), 960-966, 2017
[4] Nishiyama, Z., Martensitic transformation. 2012: Elsevier.
[5] Nakagawa, H. Miyazaki, T., Effect of retained austenite on the microstructure and mechanical properties of martensitic precipitation hardening stainless steel, Journal of materials science, 34(16), 3901-3908, 1999
[6] Bhattacharya, K., Conti, S., Zanzotto, G., Zimmer, J., Crystal symmetry and the reversibility of martensitic transformations, Nature, 428(6978), 55, 2004
[7] Coleman, A.J., Murray, K., Kearns, M., Tingskog, T.A., Sanford, B., Gonzalez, E., Properties of MIM AISI 420 via pre-alloyed and master alloy routes, in Proc. 2013 Int. Conf. Powder Metallurgy Particulate Material, Chicago, 2013

P61. A biomimetic engineered texture that turns wetting materials omniphobic even under immersion

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The search for omniphobic surfaces, which can repel all known liquids by entrapping air at the surface in a metastable (or *Cassie*) state, is of upmost importance for several industrial applications, such as water desalination, frictional drag reduction or anti-biofouling. In this field, the reliance on perfluorinated chemicals is still quite high, with several related disadvantages such as degradation under harsh conditions (temperature, chemical environment and wear) and environmental concerns. There has been thus an effort to achieve omniphobicity by using engineered surfaces, reducing the dependency on chemical coatings. Inspired by the structure of the skin of Springtails (*Collembolla*), which are soil dwelling creatures that stay dry under liquids, researchers have been designing texture-based surfaces, mostly comprised of micro-pillars with overhanging mushroom-type heads, evidencing a doubly-reentrant (DR) edge.[1] These pillar surfaces are, in fact, superomniphobic (apparent contact angles $\theta_r > 150°$), thus repelling all known liquids in drop contact angle tests. However, when these surfaces are immersed in liquids, there is a catastrophic wetting transition (from *Cassie* to *Wenzel* state) because the liquid invades the structure from the edge of the pattern (where the pillars end) of from the presence of defects. Therefore, we designed surfaces comprising DR cavities, which also entrap air in metastable state and can withstand the immersion in wetting liquids, such as water, mineral oil and hexadecane. The compartmentalized nature of the surface can also prevent the catastrophic wetting transitions, as observed in pillared surfaces, because the damaged cavities can get filled with liquid while the adjacent ones remain dry.[2] Thermodynamic equilibrium mandates that eventually the surfaces will transition from *Cassie* to *Wenzel* state, but by studying the mechanisms by which these transitions occur and the influence of cavity geometry on its kinetics, it was possible to delay the wetting transition for more than one month.[3]

References

[1] T. L. Liu and C. J. Kim, Science, **346**, 1096 (2014)
[2] E. M. Domingues, S. Arunachalam and H. Mishra, *ACS Applied Materials and Interfaces*, **9**, 21532 (2017)
[3] E. M. Domingues, S. Arunachalam, J. Nauruzbayeva and H. Mishra, *Nature Communications*, **9**, 1 (2018)

P62. Growth, structure and magnetic properties of $NdFeO_3$ single crystals

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In recent past, the research on rare-earth orthoferrites has received a renewed attention, due to their attractive properties, promising for applications in ultrafast spin switching, spin reorientation transition and multiferroics. These Properties were driven by asymmetric exchange interaction between rare-earth 4*f* and Fe-3*d* electrons . These orthoferrite have wide range of imperative technological important, recognition of high-frequency magnetization precession, stable dielectric as well as charge transport properties over a wide range of frequencies, and photocatalytic activities. In this family, $NdFeO_3$ shows a sequence of magnetic transitions in the same orthorhombic *Pbnm* perovskite structure during cooling. Below the N´eel temperature $T_N \approx 760$ K, the Fe^{3+} spins demonstrate the *G*-type antiferromagnetic (AFM) order with slight spin canting, caused by the Dzyaloshinskii- Moriya interaction, resulting in a weak ferromagnetic (FM) moment along the *c* axis.

In this work, good quality (100) oriented $NdFeO_3$ (NFO) single crystal was grown by optical floating zone method. The crystal was characterized by temperature dependent Raman spectroscopy and magnetic measurements with wide range of temperature (83 - 673 K) .Raman spectra displayed features that correspond to the perovskite structure and the modes typical to the orthorhombic *Pbnm* symmetry. The different stages of phase transition are clearly noticed in temperature dependent Raman measurement.. The temperature-dependent dielectric constant and loss tangent data measured between the frequencies of 1 kHz and 1 MHz show no anomalies around the magnetic transition temperature. In magnetic measurements a clear change of slope occurred in zero field cooled and field cooled measurements in the range 100 - 170 K and these changes correspond to the contribution of spin glass transition. Magnetic hysteresis loops displayed antiferromagnetic nature with canted spins and changes in M-H cycles can be traced to the M-T relation in the measured temperature range. The positive slope of the Arrott plots from 0 T to 10 T reveals that the antiferromagnetic-paramagnetic phase transition is second-order in nature. The magnetocaloric property of NFO single crystal was calculated and its renders that this material has potential for magnetic refrigeration in the low temperature (<50 K) range.

P63. Unusual magnetic properties of BLFO – KBr nanocomposites

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Pure and rare earth doped bismuth ferrite ($BiFeO_3$) are unique multiferroics with the large ferroelectric (FE) polarization and antiferromagnetic (AFM) order coexisting up to room and elevated temperatures.

The **purpose** of this study is to measure and analyze magnetostatic response of newly synthesized $Bi_{0.9}La_{0.1}FeO_3$ - KBr composites consisting of nanosized ferrite $Bi_{0.9}La_{0.1}FeO_3$ (BLFO) conjugated with fine grinded ionic conductor KBr. XRD and SEM were used to study the structural properties and confirm nanoscale particle sizes (≈100 nm) in the composite.

We performed **magnetostatic measurements**, which revealed that when the fraction of KBr is rather small (less than 15 wt %) the magnetic response of the composite is very weak and similar to that observed for the BLFO. When the fraction of KBr increases above 15%, the magnetic response of the composite changes substantially and the field dependence of magnetization reveals ferromagnetic-like hysteresis loop with a remanent magnetization about 0.14 emu/g and coercive field about 1.8 Tesla at room temperature. For BLFO ceramics magnetization quasi-linearly increases with magnetic field.

Different physical mechanisms were considered to explain the unusual magnetic properties of BLFO-KBr nanocomposites, and it turned out that only those among them, which are highly sensitive to the interaction of antiferromagnetic $Bi_{0.9}La_{0.1}FeO_3$ with ionic conductor KBr, can be relevant. Using Landau-Ginzburg theoretical approach we **concluded** that an appropriate mechanism turned out to be ferro-magneto-ionic coupling [1].

References

[1] D. V. Karpinsky, O. M. Fesenko, M. V. Silibin, S. V. Dubkov, M. Chaika, A. Yaremkevich, A. Lukowiak, Y. Gerasymchuk, W. Strek, A. Pakalniskis, R. Skaudzius, A. Kareiva, Y. M. Fomichov, V. V. Shvartsman, S. V. Kalinin, N. V. Morozovsky, and A. N. Morozovska. Ferromagnetic-like behavior of $Bi_{0.9}La_{0.1}FeO_3$-KBr nanocomposites. (http://arxiv.org/abs/1901.08913).

P64. Graphoepitaxial growth of CeO_2 thin films on tilted-axes $NdGaO_3$ substrates by pulsed laser deposition

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CeO_2 thin films were grown on $NdGaO_3$ tilted-axes substrates by PLD showing three-dimensional graphoepitaxial (3DGE) growth in the whole studied range of tilt angles 5-27º. Deviations from the tangent dependence can be divided into systematic negative part and local deviations near certain film tilt angles. The systematic deviation may be explained as the effect of completely-strained coherent growth of bottom layers of CeO_2 film. Minimization of the surface energy near the small-index crystallographic planes, (120) and (130), may be proposed as an explanation for the local deviations from the calculated dependence. Width of the rocking curve and lattice constant variation for the 3DGE CeO_2 films increases almost linearly with the substrate tilt angle until 19º and decrease for higher tilt angles.

The orientation and structure of the 3DGE CeO_2 films strongly depend on the deposition rate. High deposition rate generates high supersaturation at the surface of the growing film, resulting in an insufficient oxygenation of Ce ions and formation of a film with expanded lattice due to presence of oxygen vacancies in the film. An increase of the relaxation time between the laser pulses promotes oxygenation and decreases the density of oxygen vacancies in the film. At the same time, the prolonged relaxation between the laser pulses stimulates defects annealing in the film and, hence, removes the systematic deviation due to coherent seeding of the film on the substrate surface. High repetition rate, to the contrary, conserves the initial orientation through the whole film.

P65. Theoretical investigation of structural, electronic and mechanical properties of Al-doped c-BN compound

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Abstract

In the present work, we calculated structural, electronic, mechanical properties of pure and Al doped c-BN. Moreover, we report first-principle phonon frequencies and Anharmonic thermodynamic properties of pure and Al-doped c-BN within quasi-harmonic approximation, including grüneisen parameters, thermal expansion, and isobaric heat capacity. The results are discussed and analyzed.

Introduction

An extraordinary mechanical strength of cubic boron nitride (c-BN) along its high melting point and wide band gap has drawn much interest in theoretical exploration of these materials. Even though, it is softer than diamond, its superior thermal and chemical stability make it a suitable candidate for coating and high duty tools and are used in parts of high-temperature equipment's. It exists in different polytypes (c-BN, h-BN, r-BN, w-BN), among these c-BN and h-BN are analogous to diamond and graphite, respectively, and are stable at ambient conditions. c-BN with its zinc blende structure is isostructural and isoelectronic to diamond.

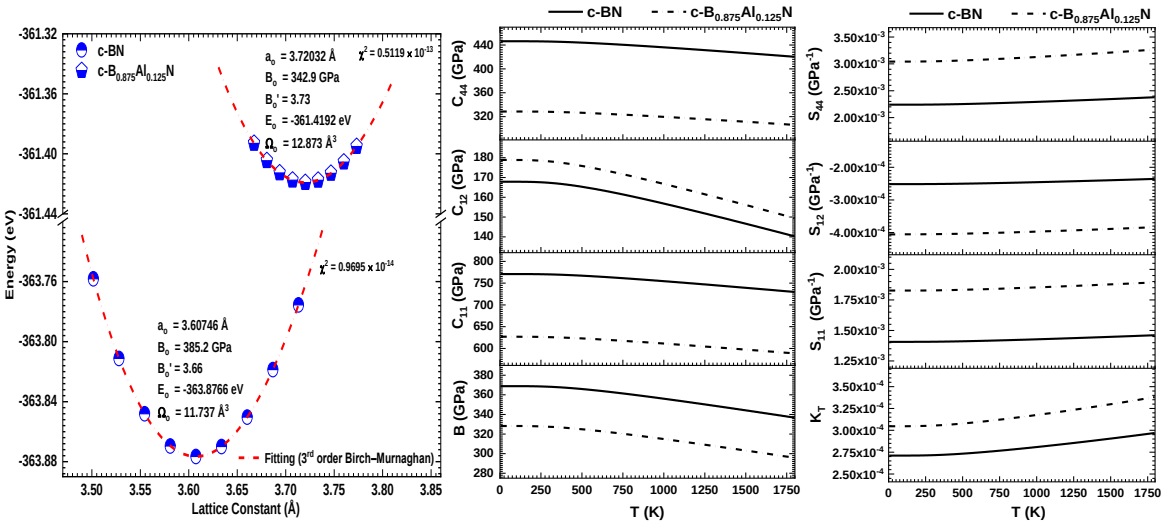
Computational Details:

The calculations were carried out within the density functional theory (DFT) framework using Quantum ESPRESSO (QE) package [1]. For testing the exchange and correlation effect, separate calculation with local density approximation (LDA) [2]as well as generalized gradient approximation (GGA) (with revised Perdew, Burke, and Ernzerhof (PBE) [3]functional for densely packed solids, PBEsol [3]) were carried out for the exchange-correlation functional. Electron-ion interaction was treated with pseudopotential method. An optimized, highly accurate non conversing pseudopotential files with valence electron configuration $2s^2 2p^1$, $2s^2 2p^3$, and $3s^2 3p^1$, for B, N, and Al atoms, respectively were directly used from pseudo-dojo library for all calculations [4]. After testing for convergence of various parameters, the kinetic energy cut-off was set to 100 Ry while the charge density cut-off was set to 400 Ry. The integration over the brillouin zone (BZ) was performed employing 18 x 18 x 18 Monkhorst–Pack (MP) k-points mesh. Checking with a more condensed k-points sampling and a larger kinetic energy cutoff in the present case did not resulted in any significant change in the ground state energy. The difference in the energy was found to be less than 0.01 meV. The atoms in the structure were fully relaxed to till all forces became smaller than 10^{-3} $eV/Å$. The energy convergence parameter was set to 10^{-8} eV . A 16 atom $2 \times 2 \times 2$ Face Centered Cubic (FCC) supercell after substituting a B atom with Al atom was used for 12.5% Aluminum (Al) doped calculation. For accurate comparison of results MP grid for 12.5% Al doped BN was reduced 2-fold to 9 x 9 x 9. The density functional perturbation theory (DFPT) as implemented in the phonon code with QE [3, 5] was used to calculate phonon frequencies on a 4 x 4 x 4 grid q-points for pure and 2 x 2 x 2 for 12.5% Al-doped BN. Fourier interpolation was used for other points in the BZ. Anharmonic properties calculation within the framework of quasi-harmonic approximation were done to obtain all

thermophysical properties of pure and 12.5% Al doped boron nitride using thermo_pw package integrated with QE- version 6.3 [6].

Conclusion

Using density functional theory and the quasi harmonic approximation, we analyzed the lattice dynamics and thermophysical property and its effect on Al doping in c-BN compound. The results is compared with experimental reports and discussed. Figure below shows a comparative structural and thermophysical behavior of pure and Al-doped c-BN.



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References

1. Journal of Physics: Condensed Matter, 2009. 21(39): p. 395502.
2. Physical Review B, 1981. 23(10): p. 5048-5079.
3. Physical Review Letters, 2008. 100(13): p. 136406.
4. Physical Review B, 2013. 88(8): p. 085117.
5. Reviews of Modern Physics, 2001. 73(2): p. 515-562.
6. https://dalcorso.github.io/thermo_pw/.
7. Physical Review, 1947. 71(11): p. 809-824.
8. Proceedings of the National Academy of Sciences, 1944. 30(9): p. 244.

P66. DFT investigation of mechanical strength of graphene and adsorption of H_2 , NO and CO on monolayer graphene and graphene oxide

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Abstract

The young's modulus of single layer graphene sheet under uniaxial strain is calculated by applying strain in 3 different configurations (isotropic strain, along zigzag direction and along armchair direction). The obtained value of the young's modulus is comparable to the experimental values. Further, 10 different configuration of monolayer graphene sheet in its functionalized form (GO) with epoxide and hydroxyl group is considered for adsorption studies. The results are discussed and analyzed.

Computational Details:

The calculations were carried out within the density functional theory (DFT) framework using Quantum ESPRESSO (QE) package [1]. All electronic calculation is done using generalized gradient approximation (GGA) exchange-correlation functional. Electron-ion interaction was treated with pseudopotential method. After testing for convergence of various parameters, the kinetic energy cut-off was set to 50. The integration over the brillouin zone (BZ) was performed employing 18 x 18 x 1 Monkhorst–Pack (MP) k-points mesh for pristine configuration. The atoms in the structure were fully relaxed to till all forces became smaller than $10^{-3}\ eV/Å$. The energy convergence parameter was set to $10^{-8}\ eV$. For physisorption studies calculation were done using rVV10 density functional for treating non local interaction between graphene layer and adsorbed molecule. The binding energy of the epoxide and hydroxyl functional groups on graphene is calculated with respect to the sum of energies of pristine graphene and isolated O and OH in vacuum as

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

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

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

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

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

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

Adsorption Study

Various configuration for GO structure were initially optimized with varying concentration of epoxide and hydroxyl group as shown in figure 2. The binding energy were calculated using equation 1 and listed in Table 1.

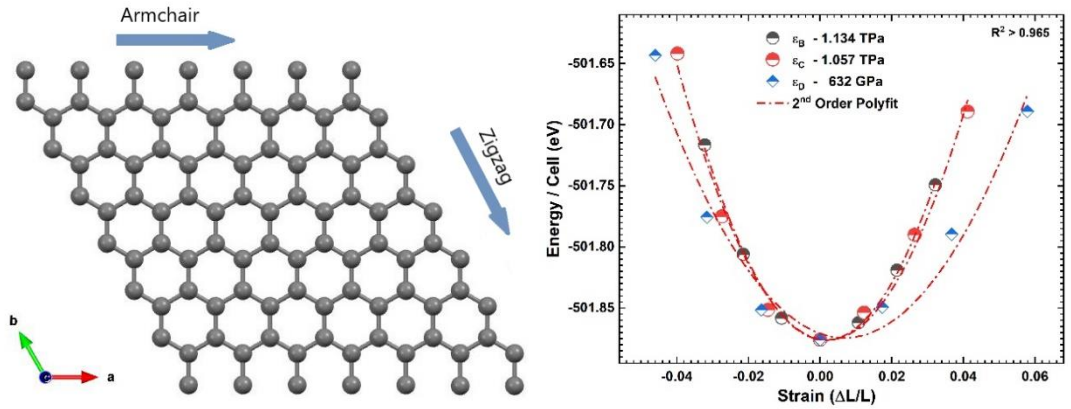

Figure 1. (a) Model of graphene sheet for calculation of mechanical property and (b) potential energy against strain for graphene sheet using DFT.

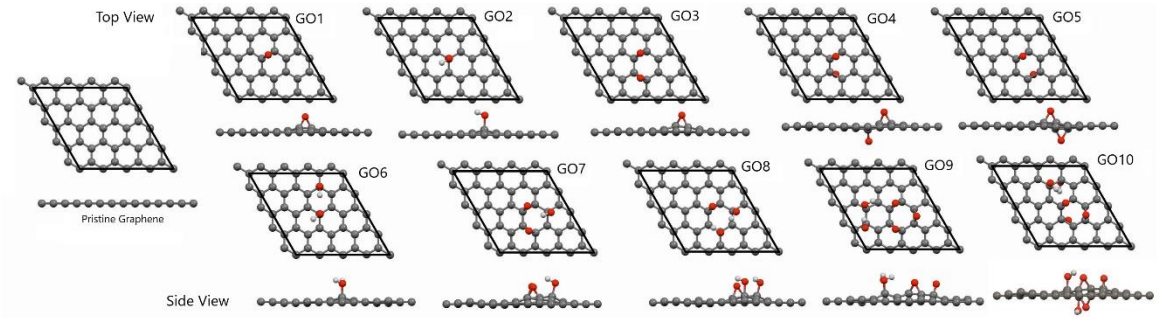

Figure 2. Optimized geometry of various configuration of Graphene Oxide for adsorption study.

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

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Reference

[1] P. Giannozzi, et al., Journal of Physics: Condensed Matter, 21 (2009) 395502.

P67. Synthesis and characterization of Double Pervoskites Halides

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The discovery of lead-free double perovskites provides a workable approach for searching air-stable and environmentally benign solar cell absorbers. The double perovskite $Cs_2AgBiCl_6$ nanoparticles was synthesized by solution route. X-ray diffraction measurements showed that the compound adopts a cubic double perovskite structure, with lattice parameters of 10.77 Å. Diffuse reflectance measurements reveal band gap of 2.77 eV that is slightly smaller than the band gap of the analogous lead halide perovskites, 3.00 eV for $CH_3NH_3PbCl_3$. The compound is stable when exposed to air. These results show that halide double perovskite semiconductors are potentially an environmentally friendly alternative to the lead halide perovskite semiconductors.

References

[1] Jun Zhou,Zhiguo Xia, Maxim S. Molokeev, Xiuwen Zhang,Dongsheng Peng, Quanlin Liua J. Mater. Chem. A, 5, 15031–15037 (2017)
[2] Eric T McClure, Molly R Ball, Wolfgang Windl, Partick M Woodward Chem. Mater., 28(5),pp1348-1354 (2016).

P68. Radiation-induced point defects transformation in irradiated lithium fluoride crystals after their mechanical fragmentation

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Influence of ionizing radiation on the dielectric crystals leads to the formation of intrinsic point defects in them, which are called radiation defects or color centers [1]. Such crystals with intrinsic radiation-induced point defects are widely used in deferent technologies, for example, as gain media in solid-state lasers [2], as detectors and dosimeters of ionizing radiation [3], as waveguides and structures with high spatial resolution [4].

Samples of LiF were studied in this work. Radiation defects were created by gamma rays from a ^{60}Co source irradiating the LiF crystals at liquid nitrogen temperature. The nanocrystals were fabricated by mechanical fragmentation of those LiF crystals. Photoluminescence measurements were carried out to establish concentration of bulk and near-cluster color centers.

It is shown that changes in the concentrations of usual radiation defects and formation of near-cluster color centers occur in nanocrystals fabricated by mechanical fragmentation of irradiated LiF crystals. Concentrations of near-cluster color centers increase to a stationary value after fragmentation and remain constant at room temperature for a long time. Influence of UV radiation on fabricated nanocrystals after termination of center formation processes in them significantly increases the concentration of F_{C3}^{+} defects.

References

[1] F. Agullo-Lopez, C.R.A. Catlow, P.D. Townsend, *Point Defects in Materials*, Academic Press Inc, San Diego (1988)

[2] T.T.Basiev, P.G.Zverev, S.B.Mirov *in Handbook of Laser Technology and Applications.* – Taylor & Francis Group, CRC Press, Philadelphia, (2003), pp. 499–522.

[3] P. Lecoq, A. Gektin, M. Korzhik *Inorganic Scintillators for Detector Systems: Physical Principles and Crystal Engineering*, Springer, Berlin, (2017).

[4] R. M. Montereali // in: H. S. Nalwa (Ed.), *Handbook of Thin Film Materials*. – Academic Press, New York, 2002, pp. 399–431.

P69. Development of 3D electrospun PCL/Chitosan scaffolds for musculoskeletal tissue engineering

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Mimic the complex cellular microenvironments in vivo of extracellular matrix (ECM), with all its essential features, it is a key challenge in tissue engineering. Three-dimensional fibrous structures (scaffolds), function efficiently as artificial ECM being therefore intensively studied in the last decades.

The fabrication of ECM analogues has been attempted with different materials and a major focus has been given to techniques. 3D printing is currently the method that has attracted the most attention because of its fast and easy production of custom shaped materials. However, as any emerging technology these additive manufacturing methods have some disadvantages: production cost is still high, post-processing is usually needed and dimensional accuracy may be of low quality.

Recently, an innovative alternative procedure to obtain 3D architectures has been reported, Thermally Induced Self-agglomeration (TISA) [1]. It is a very simple and economical technique, which allows manufacturing highly porous fibrous structures (~95%), with interconnected pores of multiple sizes. In this study, it is reported, the production nanofibers mats of polycaprolactone (PCL)/chitosan blends using acetic acid/formic, through electrospinning, and then, the conversion into 3D scaffolds using the methodology TISA, followed by freeze drying (Figure 1). The obtained scaffolds in terms of morphology, structure and properties, indicates that the produced architectures are highly promising for their application in musculoskeletal tissue engineering.

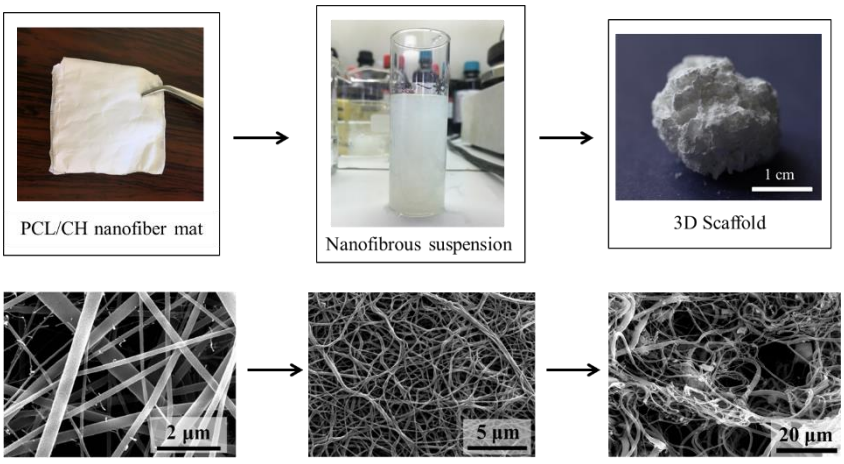

Fig. 1. *A scheme of TISA technique with SEM images of materials obtained after each step.*

References 1. T. Xu, J. M. Miszuk, Y. Zhao, H. Sun, *Adv. Healthcare Mater.* **2015**, 4, 2238-2246.

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

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

Notes

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