FUNCTIONAL MATERIALS
& NANOTECHNOLOGIES

NIBS
conference 2022
Nanotechnology | Innovation | Baltic Sea Region

Joint International Conference
Functional Materials and Nanotechnologies and
Nanotechnology and Innovation in the Baltic Sea Region

FM&NT – NIBS 2022

Riga, Latvia
July 3 – July 6, 2022

BOOK OF ABSTRACTS

INSTITUTE OF SOLID STATE PHYSICS
UNIVERSITY OF LATVIA

UNIVERSITY OF LATVIA
INSTITUTE OF
CHEMICAL PHYSICS

Edited by Līga Grīnberga, Anatolijs Šarakovskis Institute of Solid State Physics,University of Latvia 8 Ķengaraga Street, LV-1063, Riga, Latvia
E-mail: issp@cfi.lu.lv www.cfi.lu.lv

Edited by Gunta Kunakova
University of Latvia, Jelgavas str. 1, Riga
E-mail: lu@lu.lv www.lu.lv

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Welcome Message to the
FM&NT – NIBS 2022 PARTICIPANTS

Dear Colleagues,

We welcome you to the Joint International Conference **"'Functional Materials and Nanotechnologies' and 'Nanotechnology and Innovation in the Baltic Sea region'" (FM&NT - NIBS)** that is being hosted in Riga.

The FM&NT is a continuation of our annual meetings that were postponed and only interrupted in 2020 due to the epidemiological safety measures during Covid-19. It was first organized in 2006 by the Institute of Solid State Physics, University of Latvia (ISSP UL) in Riga. Since 2013 FM&NT conferences have turned over a new page – becoming a common conference of all three Baltic countries. Now it is being organized periodically by the ISSP UL, the University of Tartu, and Vilnius University.

This year, the 4th international conference NIBS 2022 is organized jointly by the University of Latvia, the University of Southern Denmark, the Kaunas University of Technology, Lithuania, and the North German Initiative Nanotechnology (NINa SH) in cooperation with Kiel University, Germany. The first NIBS conference took place in Lithuania in 2017; since then, the event has taken place in Denmark, Poland, and due to the Covid pandemic, also online. The NIBS conference brings together researchers and business stakeholders from the Baltic Sea Region to share the latest achievements in research, innovative solutions, and applications in the field of nanotechnology.

The purpose of the joint FM&NT - NIBS conference is to gather material scientists, physicists, chemists, research staff, engineers, and experts in a wide range of the most demanding application areas. Also including students from universities, research institutes, and related industrial companies. The conference topics include Optical materials; Nanocomposites and ceramics; Thin films and coatings; Energy harvesting and storage; Electronic and photonic devices, and many more. 170 different plenary sessions, invited, oral, and poster presentations of high scientific quality will be given throughout the conference. The joint event will also provide a platform for future collaboration promoting interdisciplinary research.

The FM&NT - NIBS conference will take place at the House of Science, Academic Centre of the University of Latvia in Riga. The conference dinner will be held at the Botanical Garden of the University of Latvia, which is celebrating its 100th anniversary this year.

We thank all supporters - ERDF project "The University of Latvia in the European Research Area – excellence, activity, mobility, capacity" (Project No. 1.1.1.5/18/I/016); CAMART^2 (European Union's Horizon 2020 Framework Programme H2020-WIDESPREAD-01-2016-2017-TeamingPhase2 under grant agreement No. 739508), Horizon 2020 project "CanBioSe — Novel 1D photonic metal oxide nanostructures for early stage cancer detection" (Grant Agreement No: 778157), Raith GmbH, and SIA LaboChema Latvija for making this conference happen!

Thank you all for coming, and we hope you will have the most successful and enjoyable conference!

Chairpersons of the FM&NT – NIBS 2022 conference

Dr. habil.phys. Andris Šternbergs
Institute of Solid State Physics,
University of Latvia

Prof.Dr.phys. Donāts Erts,
Institute of Chemical Physics,
University of Latvia

SCIENTIFIC TOPICS OF THE FM&NT – NIBS 2022

Nanomaterials and technologies:

Theory and modelling, progressive methods, technologies and design for production, investigation of nano: particles, tubes, composites, core-shell structures; 3-D printing, thin films and coatings

Functional Materials:

Theory and modelling, functional (inorganic, organic, and hybrid) materials for electronics and photonics

Green Energy and Environment:

Theory and modelling, perspective materials, technologies for harvesting and storage of renewable energy: hydrogen, fuel cells, batteries, photovoltaics, piezoelectric, thermoelectric, LED and OLEDs, and development of diverse energy systems.

Bioengineering materials and biotechnologies:

Theory and modelling, biomaterials, micro and nanobiotechnology, biopolymers, applications in bioengineering, biomedical engineering, and technology.

The FM&NT – NIBS 2022 conference starts with the "Motivation day", where experienced researchers will present their latest achievements and results. The next day is the "Innovation day" showing science and innovation synergy, and it will be concluded with a panel discussion 'From lab to fab. What it takes to make a business out of university research'. And last but not least is the "Young Researchers' day" where along with experienced scientists, oral presentations will be given by young researchers.

LIST OF PREVIOUS FM&NT CONFERENCES

Riga (Latvia)	2006 – 2012 annually	
Tartu (Estonia)	2013	
Riga (Latvia)	2014	Joint RCBJSF and FM&NT Symposium
Vilnius (Lithuania)	2015	
Tartu (Estonia)	2017	
Riga (Latvia)	2018	
Vilnius (Lithuania)	2021	Held online

LIST OF PREVIOUS NIBS CONFERENCES

Kaunas (Lithuania)	2017	
Sønderborg (Denmark)	2018	
Poznan (Poland)	2019	Joint NanoTech Poland 2019 and NIBS conference & expo
Hamburg (Germany)	2021	Held online

FM&NT – NIBS 2022 COMMITTEES

Conference chairs: Dr. habil. phys. Andris Sternberg, Prof. Dr. chem. Donāts Erts

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Prof. Pauls Stradins, Colorado School of Mines, USA

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Prof. Sigitas Tamulevicius, Kaunas University of Technology, Lithuania

Assoc. Prof. Jacek Fiutkowski, University of Southern Denmark, Denmark

Dr. Christian Ohrt, North German Initiative Nanotechnology, Germany

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Prof. Tomas Tamulevicius, Kaunas University of Technology, Lithuania
Dr. Rynno Lohmus, Tartu University, Estonia
Prof. Ansger Mortensen, University of Southern Denmark, Denmark

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All committees sincerely hope that the FM&NT – NIBS 2022 conference will give all participants new insights into the widespread development of functional materials and nanotechnologies, enhance the circulation of information released at the meeting, and will bring new friends, contacts, and common projects!

ORGANIZERS

UNIVERSITY OF LATVIA

INSTITUTE OF SOLID STATE PHYSICS
UNIVERSITY OF LATVIA

UNIVERSITY OF LATVIA
INSTITUTE OF CHEMICAL PHYSICS

SUPPORTERS OF THE CONFERENCE:

NATIONAL DEVELOPMENT PLAN 2020

EUROPEAN UNION
European Regional Development Fund

INVESTING IN YOUR FUTURE

ERDF project "University of Latvia and Institutes in European Research Area - Excellence, Activity, Mobility, Capacity", No: 1.1.1.5/18/I/016

CAMART²

Institute of Solid State Physics, University of Latvia as the Center of Excellence has received funding from the European Union's Horizon 2020 Framework Programme H2020-WIDESPREAD-01-2016-2017-TeamingPhase2, Grant Agreement No: 739508, project CAMART²

CANBIOSE

European Union's Horizon 2020 project "CanBioSe — Novel 1D photonic metal oxide nanostructures for early stage cancer detection", Grant Agreement No: 778157

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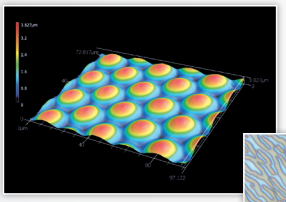
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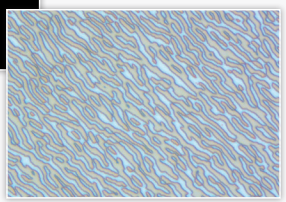
System Solutions
From Micro- to Nanofabrication

LASER





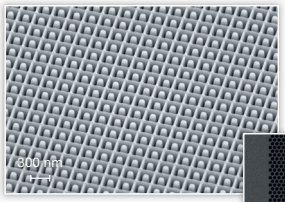
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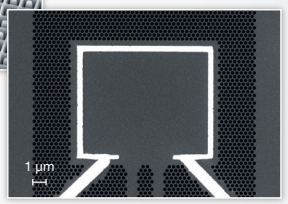
Augmented/ Virtual Reality

FIB





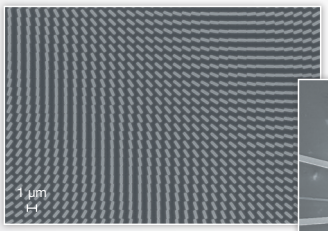
Metasurfaces



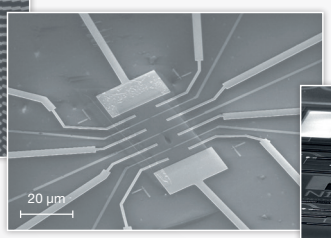
Phononic Engineering

E-BEAM

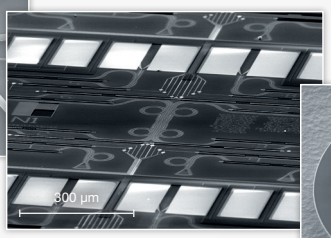




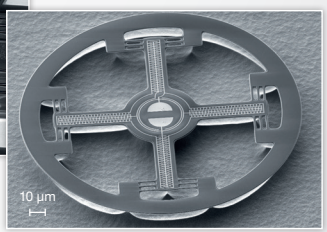
Photonics



Nanoscale Science



Quantum Technologies



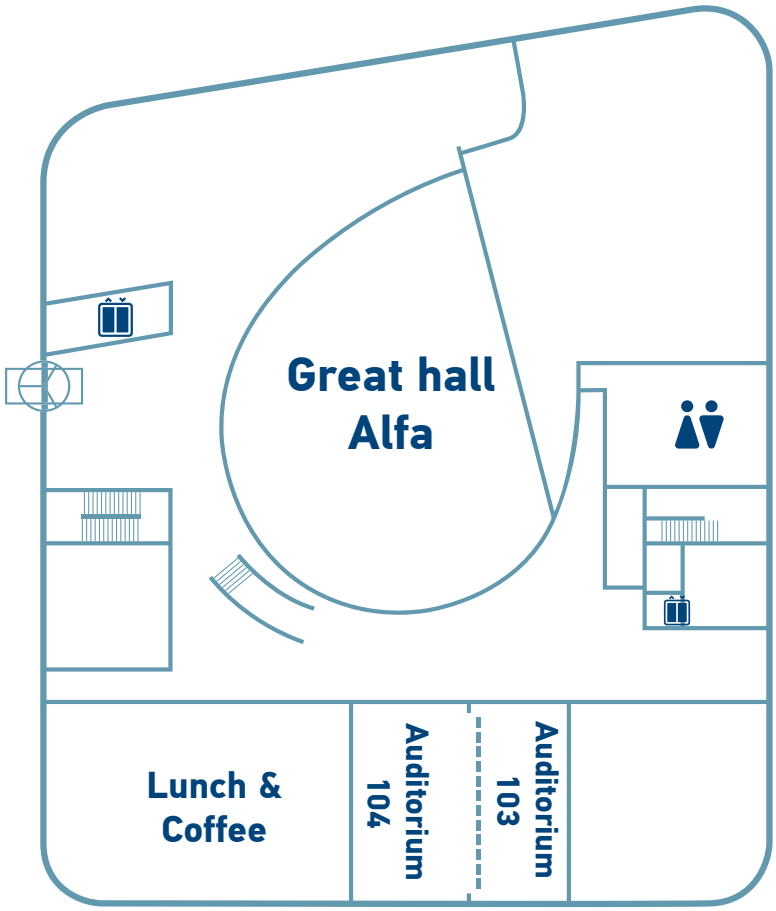
Electro-Optomechanics

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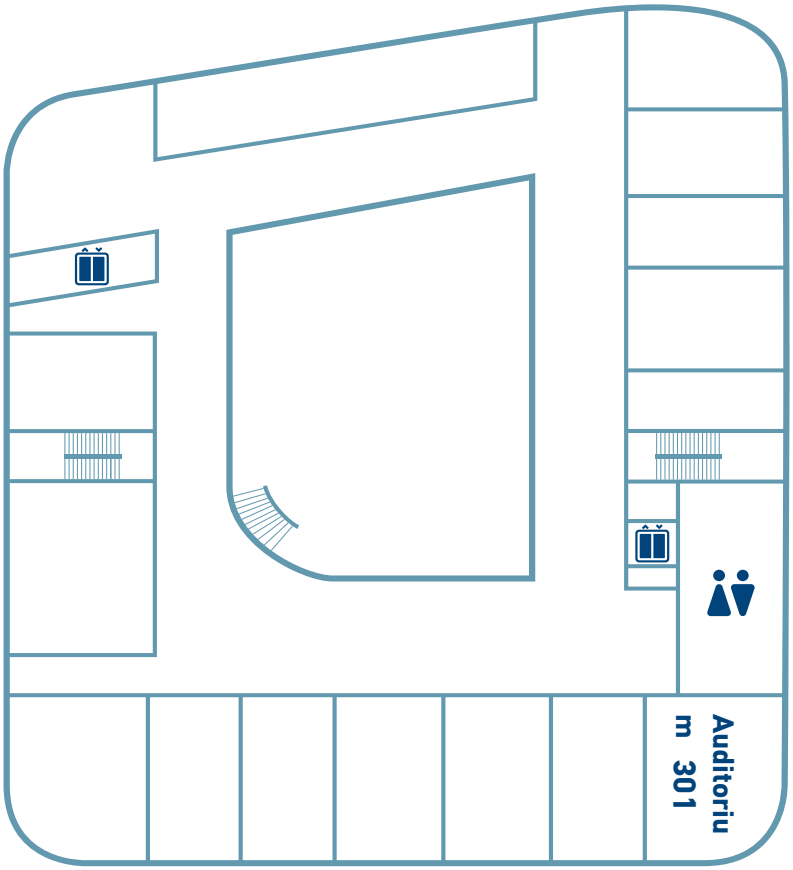
FM&NT – NIBS 2022 SITE

1st FLOOR



POSTER SESSION 2nd FLOOR ATRIUM

3rd FLOOR



FM&NT – NIBS 2022 AGENDA AT A GLANCE

July 3

16:00	**Registration**
16:00 18:00	**Welcome party**

Plenary - 40 min
Invited - 30 min
Oral - 20 min

NIBS
Biosensor materials
Functional materials (FM) - bio
Nanotechnologies
FM - properties & structure
Photonics
FM -theory & modelling
FM - For Nuclear Energy

July 4/ Motivation day

08:30	**Registration**		
	Auditorium 110 - Alfa		
09:00	**Opening** **Addresses of the conference FM&NT-NIBS 2022 representatives**		
	Chairs: Prof. Franz Faupel, Dr. Mārtiņš Rutkis		
09:20	**Anne Staubitz**		
10:00	**Muhammet S. Toprak**		
	Coffee 10:40 - 11:00		
	Prof. Franz Faupel, Prof. Anne Staubitz	*Prof. Almira Ramanavičiene*	*Dr. José Montero Amenedo*
	Aud. Alfa 110	**Aud. 103/104**	**Aud. 301**
11:00	A.-V. Mudring	S. Račkauskas	A. Ivask
11:30	A. Ramanavicius	I. Iatsunskyi	M. Bechelany
12:00	R. Meija	R. Viter	T. Tamulevičius
12:20	A. Šutka	O.Sulaieva	V. Kisand
12:40	P. Solař	M.Pogorielov	M. Tutkus
	13:00 - 14:00		
	Prof. Franz Faupel, Prof. Anne Staubitz	*Dr. prof. Jacek Fiutowski*	*Dr. Mārtiņš Rutkis*
	Aud. Alfa 110	**Aud. 103/104**	**Aud. 301**
14:00	S. Lara Avila	S. Vlassov	J. Montero-Amenedo
14:30	E. Coy	K. Staliunas	S. Woodward
15:00	M.Katkov	B. Berzina	B. Hamawandi
15:20	J. Macutkevic	H.-M. Piirsoo	J. Andžāne
15:40	J. Purāns	A. Šarakovskis	D. Wlodarczyk
	Photo & Coffee & Snacks 16:00 - 16:30		
	Poster session 16:30 - 18:30		

July 5/ Innovation day

08:30	**Registration**		
	Auditorium 110 - Alfa		
08:50	**Technical information**		
	Prof. Horst-Günter Rubahn, Prof. Marco Kirm		
09:00	**Morten Madsen**		
09:40	**Jiri Kulda**		
	Coffee 10:20 - 10:40		
	Aud. Alfa 110	**Aud. 103/104**	**Aud. 301**
	Prof. Horst-Günter Rubahn, Prof. Jacek Fiutowski	*Dr.habil. Eugene Kotomin*	*Dr. Aleksejs Kuzmins*
10:40	T. Klassen	M. Kirm	J. Banys
11:10	R. Zontovičius	G. Pucker	A. Scherz
11:40	M. Rutkis	L. Grineviciute	J. M. Kahk
12:00	G. Kucinskis	J. Grūbe	A. Guļāns
12:20	A.Ozols	R. Nedzinskas	E. Palaimiene
	Lunch 13:00 - 14:00		
	Auditorium 110 - Alfa		
	Moderator: Prof. Horst-Günter Rubahn		
14:00 - 16:00	Panel Discussion: "From lab to fab. What it takes to make business out of university research." Panelists: Romanas Zontovicius, Kaunas ST park Emil Højlund-Nielsen, CPHNano Lawrence Nsubuga, Aminic ApS Ainārs Ozols, EuroLCDs		
16:30 - 21:00	**Excursion & Conference dinner at the Botanical Garden of the University of Latvia**		

July 6/ Young researchers' day

08:30	**Registration**		
	Aud. Alfa 110	**Aud. 103/104**	**Aud. 301**
	Prof. Sigitas Tamulevičius	*Assoc.prof. Roman Viter*	*Prof. emeritus Jiri Kulda*
09:00	S. Kumar	R. Jaaniso	M. F. Hoedl
09:30	G. Kunakova	A. Ramanavičiene	E. Kotomin
10:00	C. P. Canales	J. Prikulis	D. Gryaznov
10:20	J. Szewczyk	K. Šmits	A. Česnokovs
	Coffee 10:40 - 11:00		
	Aud. Alfa 110	**Aud. 103/104**	**Aud. 301**
	Prof. Sigitas Tamulevičius, Dr. Juris Prikulis	*Prof. Tony Donné*	*Prof. Anatolijs Šarakovskis*
11:00	A. Tamulevičiene	E. Urbonavicius	S. Ubizskii
11:30	S. Schröder	A. I. Popov	K. Traskovskis
12:00	Š. Varnagiris	A. Šternbergs	A. Pidluzhna
12:20	V. Krasnenko	E. Pajuste	M. Steponaitis
12:40	L. Jasulaneca	A. Chekhovska	T. Tiirats
	Lunch 13:00 - 14:00		
	Auditorium 110 - Alfa		
	Prof. Sigitas Tamulevičius, Dr.habil. Andris Šternbergs		
14:00	**Zeynep Altintas**		
14:40	**Tony Donné**		
15:20	**Closing ceremony**		
	Goodbye refreshments 15:40 - 17:00		

PROGRAM

Sunday, July 3 - COME TOGETHER DAY

16:00	REGISTRATION		
	Auditorium 105/106		
16:00 -18:00	WELCOME PARTY & NETWORKING		

Monday, July 4 - MOTIVATION DAY

08:30 - 09:00	REGISTRATION		
	Auditorium 110 - Alfa		
09:00 - 09:20	**Opening** **Addresses of the conference FMNT-NIBS 2022 representatives**		
Chairs:	*Prof. Franz Faupel, Dr. Mārtiņš Rutkis*		
09:20 - 10:00	Anne Staubitz	Azobenzenes and diazocines for light switchable materials	PL-1
10:00 - 10:40	Muhammet S. Toprak	Development of promising nanostructured thermoelectric materials and their hybrids through sustainable chemical routes	PL-2
10:40 - 11:00	COFFEE BREAK		
	NIBS (Auditorium 110 - Alfa)		
Chairs:	*Prof. Franz Faupel, Prof. Anne Staubitz*		
11:00 - 11:30	Anja-Verena Mudring	New and improved materials for energy applications enabled by ionic liquids and deep eutectics	INV-1
11:30 - 12:00	Arunas Ramanavicius	Electrochemical methods for the development and investigation of novel materials	INV-2
12:00 - 12:20	Raimonds Meija	Electrochemistry of nanostructured Bi_2Se_3 thin films in aqueous Li and Na electrolytes	OR-1
12:20 - 12:40	Andris Šutka	Mechanisms of polymer surface charge formation and application for energy harvesting	OR-2
12:40 - 13:00	Pavel Solař	High resolution analysis of nanoparticle speed using a mechanical time-of-flight filter	OR-3
	Biosensor Materials (CanBioSe) (Auditorium 103/104)		
Chairs:	*Prof. Almira Ramanavičiene*		
11:00 - 11:30	Simas Račkauskas	Catalyst-free metal oxide nanowire growth and application	INV-3
11:30 - 12:00	Igor Iatsunskyi	Highly regular laser-induced periodic surface silicon structures modified by MXene/TiO_2 heterostructure for enhanced photodegradation	OR-4
12:00 - 12:20	Roman Viter	Structure and optical properties of $ZnFe_2O_4$/ZnO core-shell nanofibers, deposited by coaxial electrospinning	OR-5

12:20 - 12:40	Oksana Sulaieva	The role of medical laboratories in transdisciplinary research projects on biomaterials	OR-6
12:40 -13:00	Maksym Pogorielov	Conductive PCL-MXene electrospun membrane: development and biomedical evaluation	OR-7
	Functional materials - bio (Auditorium 301)		
Chairs:	*Dr. José Montero Amenedo*		
11:00 - 11:30	Angela Ivask	Nanomaterial-based surfaces - promising alternatives to antimicrobial applications	INV-4
11:30 - 12:00	Mikhael Bechelany	Functional nanomaterials for biosensor and bone regeneration	INV-5
12:00 - 12:20	Tomas Tamulevicius	Laser-made metal nanoparticles for SARS-CoV-2 related applications	OR-8
12:20 - 12:40	Vambola Kisand	Antimicrobial activity of commercial photocatalytic SaniTise window glass	OR-9
12:40 - 13:00	Marijonas Tutkus	Super-resolution microscopy and the soft DNA curtains: high-throughput SM method for protein-DNA interaction studies	OR-10
13:00 - 14:00	LUNCH		
	NIBS (Auditorium 110 - Alfa)		
Chairs:	*Prof. Franz Faupel, Prof. Anne Staubitz*		
14:00 - 14:30	Samuel Lara Avila	Graphene for sensors and (quantum) electronics	INV-6
14:30 - 15:00	Emerson Coy	Large Applicability of Polydopamine Coatings in Energy Production	INV-7
15:00 - 15:20	Mikhail Katkov	Nitrogen-doped MWCNTs with temperature stable thermoelectric sensitivity	OR-11
15:20 - 15:40	Jan Macutkevic	Synergy effects in hybrid epoxy composites with carbon and magnetic nanoinclusions	OR-12
15:40 - 16:00	Juris Purāns	X-ray absorptions study of chromogenic materials for smart windows	OR-13
	Nanotechnologies (Auditorium 103/104)		
Chairs:	*Dr. prof. Jacek Fiutowski*		
14:00 - 14:30	Sergei Vlassov	Manipulation and characterization of individual nanostructures	INV-8
14:30 - 15:00	Kestutis Staliunas	Nanostructures for intracavity spatial filtering in microlasers	INV-9
15:00 - 15:20	Baiba Bērziņa	Aluminum nitride – persistent luminescence material	OR-14
15:20 - 15:40	Helle-Mai Piirsoo	Influence to hardness of alternating sequence of atomic layer deposited harder alumina and softer tantala nanolaminates	OR-15
15:40 - 16:00	Anatolijs Šarakovskis	Upconversion luminescence in erbium doped transparent oxyfluoride glass ceramics	OR-16

	Functional materials - properties (Auditorium 301)		
Chairs:	*Dr. Mārtiņš Rutkis*		
14:00 - 14:30	José Montero Amenedo	Multifunctional chromogenic and transparent conducting oxide nanocoatings	INV-10
14:30 - 15:00	Simon Woodward	Organic-composite thermoelectrics: balancing performance, sustainability and ease of synthesis	INV-11
15:00 - 15:20	Bejan Hamawandi	Nanostructured thermoelectric materials synthesized via solution chemical routes	OR-17
15:20 - 15:40	Jana Andžāne	Application of nanostructured materials for flexible thermoelectrics and energy-efficient buildings	OR-18
15:40 - 16:00	Damian Wlodarczyk	Novel double perovskites and their derivatives hosting rare-earth ions – a prelude to charge transfer phenomenon	OR-19
16:00 - 16:30	PHOTO, COFFEE, AND SNACKS		
16:30 - 18:30	**POSTER SESSION**		

Tuesday, July 5 - INNOVATION DAY

08:30 - 08:50	REGISTRATION		
	Auditorium 110 - Alfa		
08:50 - 09:00	**Technical Information**		
Chairs:	*Prof. Horst-Günter Rubahn, Prof. Marco Kirm*		
09:00 - 09:40	Morten Madsen	Organic photovoltaics: from thin film synthesis to large scale manufacturing	PL-3
09:40 - 10:20	Jiri Kulda	From molecular dynamics simulations to diffuse scattering maps	PL-4
10:20 - 10:40	COFFEE BREAK		
	NIBS (Auditorium 110 - Alfa)		
Chairs:	*Prof. Horst-Günter Rubahn, Prof. Jacek Fiutowski*		
10:40 - 11:10	Thomas Klassen	Hydrogen storage: from nano materials to components	INV-12
11:10 - 11:40	Romanas Zontovičius	Evolut 4.0 accelerator by Kaunas STP	INV-13
11:40 - 12:00	Mārtiņš Rutkis	Story how useless thin film thermoelectric generator become ultra-fast laser power sensor	OR-20
12:00 - 12:20	Gints Kučinskis	Preparation and characterization of electrodes for Na-ion batteries: $Na_2FeP_2O_7$ and $Na_{0.67}MnO_2$	OR-21
12:20 - 12:40	Ainārs Ozols	What silica-based thin films could do for augmented reality displays?	OR-22
	Nanotechnologies - photonics (Auditorium 103/104)		
Chairs:	*Dr.habil. Eugene Kotomin*		
10:40 - 11:10	Marco Kirm	A band structure engineering concept applied in design of novel light emitting materials	INV-14
11:10 - 11:40	Georg Pucker	Silicon micro and nanofabrication in the context of quantum optics	INV-15

11:40 - 12:00	Lina Grinevičiute	Nanostructured anisotropic multilayer coatings for the manipulation of laser radiation	OR-23
12:00 - 12:20	Jurģis Grūbe	Photolithography utilizing up-conversion luminescence in nanoparticles mixed with SU8 photoresist with/without organic compounds	OR-24
12:20 - 12:40	Ramūnas Nedzinskas	Optical spectroscopy of high-quality ZnO (0002) / Cu (111) thin films grown by electrodeposition	OR-25
	Functional materials - structure (Auditorium 301)		
Chair:	*Dr. Aleksejs Kuzmins*		
10:40 - 11:10	Juras Banys	Phase transitions in metal organic frameworks	INV-16
11:10 - 11:40	Andreas Scherz	Ultrafast material dynamics studies at the European XFEL	INV-17
11:40 - 12:00	Juhan Matthias Kahk	Computational methods for guiding peak assignment in X-ray photoelectron spectroscopy	OR-26
12:00 - 12:20	Andris Guļāns	Impact of spin-orbit interaction on structure of materials	OR-27
12:20 - 12:40	Edita Palaimiene	ALN ceramics ferroelectric properties and phase transitions dynamics	OR-28
13:00 - 14:00	LUNCH		
	Auditorium 110 - Alfa		
14:00 - 16:00	Panel Discussion: "From lab to fab. What it takes to make business out of university research." Moderator: Prof. Horst- Günter Rubahn, University of Southern Denmark Panelists: Romanas Zontovičius, Kaunas ST park, Emil Højlund-Nielsen, CPHNano, Lawrence Nsubuga, Aminic ApS Ainārs Ozols, EuroLCDs		
16:00 - 16:30	GATHERING FOR THE EXCURSION BUSS		
16:30-21:00	EXCURSION & CONFERENCE DINNER		

Wednesday, July 6 - YOUNG RESEARCHERS' DAY

08:30 - 09:00	REGISTRATION		
	NIBS (Auditorium 110 - Alfa)		
Chairs:	*Prof. Sigitas Tamulevičius*		
09:00 - 09:30	Shailesh Kumar	On-chip source of polarized single photons with orbital angular momentum	INV-18
09:30 - 10:00	Gunta Kunakova	Charge transport in topological insulator nanostructures	INV-19
10:00 - 10:20	Camila Pía Canales	The decade of hydrogen: where are we heading to?	OR-29
10:20 - 10:40	Jakub Szewczyk	Application of biomimetic polydopamine 2D-like thin films for a significant enhancement of ZnO and TiO_2 photocatalytic properties	OR-30

	Biosensor materials (CanBioSe) (Auditorium 103/104)		
Chairs:	*Assoc.prof. Roman Viter*		
09:00 - 09:30	Raivo Jaaniso	Graphene-based sensors for environmental monitoring	INV-20
09:30 - 10:00	Almira Ramanavičienė	Magnetic gold-coated nanoparticles for bioanalytical application	OR-31
10:00 - 10:20	Juris Prikulis	Self-organized nanostructured metal and metal oxide containing multilayers for optical sensing	OR-32
10:20 - 10:40	Krišjānis Šmits	Structural and optical properties of oxide nanoparticles and nanostructures	OR-33
	Functional materials - Theory & modelling (Auditorium 301)		
Chairs:	*Prof. emeritus Jiri Kulda*		
09:00 - 09:30	Maximilian F. Hoedl	First-principles study of proton diffusion in $BaFeO_{3-\delta}$	INV-21
09:30 - 10:00	Eugene Kotomin	First principles calculations of radiation defect properties in complex oxide crystals	INV-22
10:00 - 10:20	Denis Gryaznov	Ab-initio modelling elucidates materials trends for electrochemistry applications	OR-34
10:20 - 10:40	Andrejs Česnokovs	A first-principles study of point defects and electronic conductivity in ZnO	OR-35
10:40 - 11:00	COFFEE		
	NIBS (Auditorium 110 - Alfa)		
Chairs:	*Prof. Sigitas Tamulevičius, Dr. Juris Prikulis*		
11:00 - 11:30	Asta Tamulevičienė	SERS using self-assembled nano structures of different geometry. special case of wires, spheres and triangles	INV-23
11:30 - 12:00	Stefan Schröder	The initiated chemical vapor deposition of tailored polymer thin films - Fundamentals to advanced functional applications	INV-24
12:00 - 12:20	Šarunas Varnagiris	Plasma treatment application for green hydrogen production via hydrolysis of waste aluminum in alkaline water	OR-35
12:20 - 12:40	Veera Krasnenko	Raman vibrational spectrum modeling of water splitting on multifaceted perovskite nanoparticles	OR-36
12:40 - 13:00	Liga Jasulaneca	Cryogenic temperature nanoelectromechanical switch	OR-37
	FM&NT (For NucEnerg) (Auditorium 103/104)		
Chairs:	*Prof. Tony Donné*		
11:00 - 11:30	Egidijus Urbonavičius	Nuclear fusion research in Lithuania – history and perspectives	INV-25
11:30 - 12:00	Anatoli I. Popov	Deep understanding of advanced optical and dielectric materials for fusion diagnostic applications	INV-26
12:00 - 12:20	Andris Šternbergs	Energy and sustainability: progress in renewables and advanced “green” nuclear energetics	OR-38
12:20 - 12:40	Elīna Pajuste	Fuel retention in ITER-Like-Wall JET plasma facing components	OR-39
12:40 - 13:00	Anastasiia Chekhovska	Experimental studies of the 112Sn(g,n)111Sn and 112Sn(g,p)111m,gIn reactions for p-nuclei production simulation	OR-40

	FM - photonics (Auditorium 301)		
Chairs:	*Prof. Anatolijs Šarakovskis*		
11:00 - 11:30	Sergii Ubizskii	Hyperbolic phosphorescence decay kinetics: empirical formula and theoretical models	INV-27
11:30 - 12:00	Kaspars Traskovskis	Carbene-metal amides: an emerging class of highly efficient OLED emitters	INV-28
12:00 - 12:20	Anna Pidluzhna	Diethynyl Fluorenes as promising heavy-metal free emissive materials	OR-41
12:20 - 12:40	Matas Steponaitis	Sb_2S_3 Solar cells with cost-effective hole transport materials for semi-transparent applications	OR-42
12:40 - 13:00	Tauno Tiirats	Thermal, mechanical, and acoustic properties of polydimethylsiloxane filled with hollow glass microspheres	OR-43
13:00 - 14:00	LUNCH		
	Auditorium 110 - Alfa		
Chairs:	*Prof. Sigitas Tamulevičius, Dr.habil. Andris Šternbergs*		
14:00 - 14:40	Zeynep Altintas	Biosensor applications of functional polymers	PL-5
14:40 - 15:20	Tony Donné	Why don't we have fusion yet?	PL-6
15:20 - 15:40	CLOSING OF THE CONFERENCE		
15:40 - 17:00	GOODBYE REFRESHMENTS		

POSTER PRESENTATIONS

FUNCTIONAL MATERIALS		
Po-1	Sami Vuori	Detection of x-ray doses with color-changing hackmanites: mechanism and application
Po-2	Cecilia Agamah	Synthesis of Highly Photochromic Hackmanite from Natural Nepheline
Po-3	Guna Doke	Novel broadband near-infrared emitting long afterglow phosphor $MgGeO_3$: Cr^{3+}
Po-4	Georgijs Bakradze	Peculiarities of the local structure in a new high-entropy low-symmetry (MnCoNiCuZn)WO_4 tungstate oxide
Po-5	Jekabs Cirulis	Structure and stability of radiation defects in $LiYF_4$
Po-6	Tomas Klinavičius	Design of Antireflective Structures for the Optical Wavelength Range
Po-7	Dace Nilova	Ultraviolet long-lasting luminescence of $Ca_2Al_2SiO_7$:Pr^{3+}
Po-8	Robertas Grigalaitis	Dielectric properties of mixed halide perovskites
Po-9	Haralds Ozols	Enhancement and origin of photochromism in $BaMgSiO_4$:Fe
Po-10	Yaroslav Zhydachevskyy	Trapping, recombination and glow mechanisms in YAP:Mn^{2+} crystals as promising TL/OSL detectors
Po-11	Leonid Rusevich	Computer modelling of water splitting on perovskite nanoparticles
Po-12	Arturs Zarins	Effects of sample preparation methods on luminescence of lithium orthosilicate-lithium metatitanate ceramic pellets
Po-13	Halil Arslan	Reactive e-beam evaporation of yttrium:A spectral and structural investigation of yttrium oxide and oxyhydride thin film
Po-14	Julija Grigorjevaite	Optical properties investigation of $K_2Gd(PO_4)(WO_4)$:20%Yb^{3+} as a function of Tm^{3+} concentration
Po-15	Ernests Einbergs	Mechanical stress visualization of additively built (3D printed) objects using mechanoluminescence
Po-16	Laima Trinkler	Optical properties of ZnMgO epilayers grown on $ScAlMgO_4$ substrate
Po-17	Matas Steponaitis	No doping? No problem. Low cost carbazole enamines for efficient perovskite solar cells
Po-18	Jevgenijs Gabrusenoks	Optical properties of Cu_2O single crystals and thin films
Po-19	Andis Poļaks	Fluorine doped tin oxide work function measurements using photoelectron emission yield spectroscopy
Po-20	Meldra Kemere	Luminescence properties and energy transfer in Dy^{3+}/Eu^{3+} and Tb^{3+}/Eu^{3+} doped oxyfluoride glasses and glass-ceramics
Po-21	Blessing Adejube	Collective Functionality of Resistive Switching in Nanoparticle Assemblies
Po-22	Edvards Strods	Ga_2O_3 thin films deposited by liquid metal target sputtering
Po-23	Sergejus Balčiūnas	Dielectric properties of [NH4][Zn(HCOO)3] metal formate framework doped with alkali metals
Po-24	Augustas Vaitkevičius	Macro- and micro-scale inhomogeneities in heavily doped gadolinium aluminum gallium garnet scintillator

Po-25	Pavels Rodionovs	Red and infrared luminescence in Cr^{3+} doped calcium aluminates with different Ca/Al content
Po-26	Martynas Kinka	Broadband dielectric investigation of PEBA/UIO-66 mixed matrix membranes
Po-27	Martins Zubkins	Optical properties of high-quality ZnO / SiO_2 thin films grown by magnetron sputtering
Po-28	Monika Jokubauskaitė	Optical spectroscopy of rock-salt Zn(x)Mg(1-x)O thin films with high (up to 85%) Zn content
Po-29	Alexander Molnar	Optimization of the chemical composition of $CuInP_2S_6$ layered crystals for energy harvesting applications
Po-30	Yuriy Hizhnyi	Computational studies of atomic and electronic structures of "oxide crystal - oxide glass" interphases
Po-31	Raitis Grzibovskis	Photoelectrical properties of novel hole transport materials for semi-transparent solar cells
Po-32	Roberts Olins	Synthesis and use of functionalized graphene materials for energy storage
Po-33	Vitalii Liubachko	The appearance of the flexoelectric coupling near the ferrielectric phase transition in $CuInP_2S_6$ layered crystals
Po-34	Vanda Voikiva	Optimization of keratin extraction method from sheep wool
Po-35	Viktors Vibornijs	Tungsten oxide, copper and zinc containing anti-microbial thin film magnetron sputtering.
Po-36	Martin Lind	Assessing The Performance of Graphene-Based Gas Sensors in Ambient Air
Po-37	Ciro Federico Tipaldi	Lattice dynamics and Raman and infrared reflectance spectra of $YAlO_3$
Po-38	Gundars Strīķis	Role of nucleation layer in MOCVD growth of β-Ga_2O_3 thin films
Po-39	Juhan Saaring	Time-resolved luminescence studies of ternary hexafluorides under synchrotron radiation excitation
Po-40	Barbara Garbarz-Glos	Preparation and electric characterization of lead-free ferroelectric ceramics based on sodium-potassium niobate
Po-41	Irina Tepliakova	ZnO-Schiff base composites for optical detection of coper ions
Po-42	Aleksandrs Začinskis	Iridium incorporation defects in gallium oxide: Ab-initio simulations.
Po-43	Astrida Berzina	Neoprene and ethylene-octene copolymer composites for temperature self-regulating heating elements
Po-44	Madara Leimane	Luminescence and electron paramagnetic resonance of carbon-doped silica glass
Po-45	Maximilian F. Hoedl	The orbital nature of electron holes in $BaFeO_{3-\delta}$ and implications for defect chemistry
Po-46	Ernests Tropiņš	Optical writing in the structure of negative SU8 photoresist using up-conversion luminescence of Yb^{3+} and Tm^{3+} activated nano-particles
Po-47	Nikolay Ogurtsov	Chemiresistive gas sensors based on the core-shell nanocomposites of the conducting polymer
Po-48	Tetiana Samoilenko	UV-Curable Polymer Materials for Coating and On-Site Repair of Photovoltaic Modules of Solar Cells
Po-49	Lyudmila Kosyanchuk	New laser materials based on polyurethane with chemically bonded polymethine dye
Po-50	Nataliia Davydenko	Stabilized carbon nanotube/polypyrrole nanocomposite for VOC detection

Po-51	Iryna Myroniuk	The effect of polyaniline content on the gas sensing properties of conducting halloysite–polyaniline nanocomposites
Po-52	Olga Slisenko	Structure and transport parameters of binary polyacrylic acid / polysiloxane hybrids
Po-53	Natalia Babkina	Transparent polyurethane materials with effective damping ability and ultraviolet protection
Po-54	Paula Iesalniece	Preparation of magnesium alloy AZ31 corrosion protection coatings by combining PEO and spray pyrolysis methods
Po-55	Halyna Klym	Physical and chemical water-sorption processes in the $MgAl_2O_4$ ceramics
NANOMATERIALS AND TECHNOLOGIES		
Po-56	Aušrinė Jurkevičiūtė	Modelling of the Scattering Spectrum of Metal Nanoparticles on Porous Anodized Aluminium Oxide of Various Thickness
Po-57	Mindaugas Ilickas	Comparison of different coatings techniques for zinc oxide nanoparticles for room-temperature UV sensors
Po-58	Šarūnas Jankauskas	Synthesis of Graphene on Si(100) Using Direct MW-PECVD and protective enclosures
Po-59	Syed Shabhi Haider	Designing of Experimental Setup for Impact Induced Mechanoluminescence Measurements
Po-60	Dr Vera Skvortsova	Preparation and tribological properties of multilayer tungsten oxide nano smart coatings
Po-61	Inga Pudza	The use of tungstate nanoparticles in hybrid X-ray detectors
Po-62	Rihards Ruska	Luminescence of doped AlN materials
Po-63	Boris Polyakov	Different strategies for GaN-MoS_2 and GaN-WS_2 core–shell nanowire growth
Po-64	Kevon Kadiwala	Thin films of WSe_2 synthesized via selenization of WO_x and W precursor materials for comparison
Po-65	Marina Tretjak	Low frequency noise characteristics of composites with MWCNT and Ni@C nanoparticles
Po-66	Elza Dzene	Comparison of methods for integration of Bi_2Se_3 nanowires in NEM switches
Po-67	Gazy Khatmi	Femtosecond laser ablation at 1030 nm, second harmonic and third harmonic for Nitrocelluece membrane
Po-68	Paniz Vafaei	Graphene gas sensors grafted with TiO_2 nanolayers: temperature dependence of NO_2 response
Po-69	Sanu Bifal Maji	Time Resolved Luminescence study of Pr^{3+} doped $LuPO_4$ nanocrystals synthesized in aqua-organic solvent.
Po-70	Daniel Aguilar Ferrer	Study of the Rhodamine 6G Photodegradation Efficiency with Different Polydopamine Shell Thickness Au/PDA Nanoplatforms
Po-71	Lina Mikoliunaite	Fast Microwave Assisted Solvothermal Synthesis of Magnetite Nanospheres
Po-72	Vitalijs Lazarenko	Nanostructured Bi_2Se_3 thin films as a perspective anode for aqueous rechargeable lithium-ion batteries
Po-73	Irina Oliseveca	Investigation of Single walled carbon nanotube network anode in aqueous LiNO3 electrolyte
Po-74	Raimonds Meija	Electrochemistry of nanostructured Bi_2Se_3 thin films in aqueous Na electrolyte
Po-75	Krisjanis Buks	Properties and applications of blended and encapsulated bismuth selenide and CNT hybrid structure-based flexible thermoe
Po-76	Mati Kook	Chemical Exposure and Abrasion Effect on Photocatalytical Activity of Antibacterial Surfaces Covered with Acrylic Matrix

Po-77	Lasma Bugovecka	Mechanical stability of MWCNT and Bi_2Se_3 Thermoelectric Polymer Composite Thin Films
Po-78	Viktoriia Fedorenko	Role of polymer to forming of Fe_3O_4/Fe_2TiO_5 core-shell nanofibers, deposited by coaxial electrospinning
Po-79	Andrei Felsharuk	Fe-nanoparticle seeded growth of Bi_2Se_3 nanoribbons
Po-80	Jurij Grechenkov	Calculated optical properties of chalcopyritic solid solutions for photovoltaic applications
Po-81	Yelyzaveta Rublova	Effect of the cations on the SEI layer formation on the Bi_2Se_3 anode in aqua mediums
Po-82	Edgars Vanags	Determination of light element content in sodium bismuth titanate samples using secondary electron hyperspectral imaging
Po-83	Annamarija Trausa	SERS substrates based on gold nanoparticle-coated ZnO tetrapods
Po-84	Didzis Salnājs	Optimal synthesis parameters and characterization of catalyst-free grown Bi2Se3 nanoribbons
Po-85	Liga Bikse	Towards surface-enhanced Raman spectroscopy on the tip of optical fiber: comparison of substrates
Po-86	Nadzeya Khinevich	SERS-active substrates based on silver nanoparticle array induced surface lattice resonance
Po-87	Liga Jasulaneca	Cryogenic temperature nanoelectromechanical switch
Po-88	Loreta Brauna	Impact of electrodes on properties of flexible encapsulated Bi_2Se_3/CNT hybrid network materials
Po-89	Margarita Baitimirova	Application of graphene for enhancement of physical properties of Bi_2Se_3 and Bi_2Se_3/ZnO nanostructures
Po-90	Yana Suchikova	The technological features of nanostructures formation on the surface of indium phosphide by electrochemical etching
Po-91	Mantas Mikalkevičius	Influence of femtosecond laser parameters for imposing laser-induced periodic surface structures on silicon surface
Po-92	Pavlo Golub	Topological defects movement control in liquid crystal cells
Po-93	Davis Gavars	Thermoelectric Properties of Copper Oxide Nanowire Networks
Po-94	Halil Arslan	Reactive e-beam evaporation of yttrium: A spectral and structural investigation of the growth kinetics
Po-95	Raitis Sondors	Effect of thermally dewetted Au nanoparticles on the morphology of Bi_2Se_3 nanoribbons synthesized by physical vapor deposition
Po-96	Harleen Kaur	Optimization of conditions for testing the efficacy of antimicrobial surfaces
Po-97	Elina Neilande	Evaluation of antibacterial properties of Cu-doped titanium dioxide using DFT calculations
Po-98	Aleksandrs Dutovs	In-situ optical control of nanoporous alumina layer thickness
Po-99	Uldis Malinovskis	Sensing of vascular endothelial growth factor-A using close packed Au nanoparticle arrays on porous anodic aluminum oxide-Al templates.
Po-100	Anatolijs Truhins	Luminescence, XPS and Raman of crystalline quartz affected to high pressure by detonation
Po-101	Valerii Malyshev	Infiltration control of highly ordered nanoporous aluminum oxide membranes with aqueous electrolytes

GREEN ENERGY AND ENVIRONMENT		
Po-102	Julija Lukasevica	EXAFS study of NiO lattice dynamics using reverse Monte Carlo and force field methods
Po-103	Vitalijs Dimitrijevs	EXAFS study of lattice dynamics in metals with cubic and hexagonal structures using the reverse Monte Carlo method
Po-104	Alexei Kuzmin	Direct observation of crystal field splitting in tungstates by resonant X-ray emission spectroscopy
Po-105	Liga Britala	Inert Coatings for Cycle Life Extension of Cathodes for Li-Ion Batteries
Po-106	Ansis Mezulis	On the efficiency of hydrogen production from plasma-treated aluminum waste with NaOH and KOH promoters
Po-108	Julija Hodakovska	Analysis of Lithium Iron Phosphate Service Life in Li-ion Batteries at Different Temperatures and Cycling Rates
Po-109	Martins Vanags	Amphoteric decoupled water electrolysis for hydrogen production
Po-110	Vera Serga	Leaching of valuable metals from scrap printed circuit boards under the action of alternating current
Po-111	Raitis Kaspars Sika	Reactor design investigation for Hydrogen production from Aluminium -Water reaction
Po-113	Ainars Knoks	Electrochemical Corrosion Behavior of Aluminum Foil – investigation of kitchen wastes
Po-114	Ervīns Blumbergs	Application of the disintegration grinding method to increase the efficiency of the processing of used printed circuit b
Po-115	Yuriy Noskov	Halloysite/polyaniline nanocomposites for removal of dyes and dichromate potassium from water
BIOENGINEERING MATERIALS AND BIOTECHNOLOGIES		
Po-116	Mart Ernits	Stealthy magnetic liposomes for drug delivery
Po-117	Vladlens Grebņevs	Amorphous calcium phosphate suspensions as a way to attain bioactivity of PEO coatings
Po-118	Ott Rebane	Time-resolved fluorescence to determine the viability of bacterial spores

PLENARY

AND INVITED SPEAKERS



e-mail: astaubitz@oc.uni-kiel.de

Prof. Dr. Anne Staubitz
Institute for Organic and Analytical Chemistry, University of Bremen
Germany

Anne Staubitz holds a post as a professor at the University of Bremen. Her interests are the development of nucleophile selective cross-coupling reactions and, using this tool, the synthesis of new semiconducting polymers. A second research thrust has developed within the collaborative network CRC 677 "Function by Switching", which is concerned with switchable polymeric systems and their application in materials science. This research is still conducted at Kiel University where Anne Staubitz has a part-time associate professorship. Anne Staubitz studied biochemistry at the University of Tübingen. After working in Paul Knochel's group at the University of Munich (LMU) on novel Grignard reagents, she obtained her Ph. D. with Varinder Aggarwal at the University of Bristol, UK, working on a natural product. For her post-doctoral work she joined the group of Ian Manners, also at the University of Bristol, where she worked on main group inorganic polymers, in particular catalytic dehydrocoupling reactions of group 13 group 15 adducts. She started her independent academic career as an assistant professor at Kiel University in 2010, and continues to contribute to the CRC 677.



e-mail: toprak@kth.se

Prof. Muhammet S. Toprak
Royal Institute of Technology (KTH)
Sweden

Muhammet S. Toprak received his B.Sc. in Chemistry Education and M.Sc. in Inorganic Chemistry from the Middle East Technical University (METU, Ankara-Turkey). During the PhD studies at METU he moved to Sweden and completed his PhD in Materials Chemistry at KTH - Royal Institute of Technology (Stockholm-Sweden), specializing in Inorganic Materials Chemistry and Nanotechnology. He worked as a Post-doctoral fellow at the University of California at Santa Barbara (UCSB, USA) on the biomimetic assembly routes for the fabrication of nanomaterials. He then returned to KTH and received the title of Docent in 2009, thereafter was appointed full Professor in Materials Chemistry in 2015. He is currently a staff member at the Department of Applied Physics, KTH, leading a research group with a strong Nanochemistry profile. Material design on the nanoscale is Toprak's main research domain. The focus is on developing sustainable methods (green chemistry) for synthesizing nanomaterials with controlled size, morphology and surface chemistry (nanotectonics), precisely engineered for the intended applications. Toprak's research activities have a strong sustainability focus, with a special emphasis on applications in energy and biomedicine. Thermoelectric materials are one area where his group has a strong track-record, reporting several materials displaying state-of-the-art performance. The aim is scalable hybrid materials for thermal energy harvesting. For biomedicine, the group developed nanoparticles with biocidal and bio-active surfaces. A pioneering area is the development of a library of novel nanoparticle-based contrast agents, and demonstration of the usability of the new contrast agents for in-vivo x-ray fluorescence bio-imaging. Development of targeted nanoparticle delivery in-vivo is the objective of on-going research. He has published more than 250 articles in internationally renowned journals and have an h-index of 61. His research has been supported by the major funding agencies such as the Swedish Research Council, Swedish Energy Agency, the Knut and Alice Wallenberg Foundation, Vinnova, and the European Commision through FP7-H2020 programs.



e-mail: madsen@mci.sdu.dk

Prof. Morten Madsen
University of Southern Denmark, Mads Clausen Institute, NanoSYD
Denmark

Professor at University of Southern Denmark, the Mads Clausen Institute and head of SDU Centre for Advanced Photovoltaics and Energy (SDU CAPE). My field of expertise is thin-film growth, integration and devices for energy conversion and storage applications. In 2010-2011, I worked with high performance transistors from III-V nanoscale membranes at the Javey research lab, UC Berkeley, California. In 2011, I established the OPV group at SDU NanoSYD, where we work on improving the performance and stability of organic and hybrid solar cells, including thin film synthesis, metal oxide interlayers and interfaces, organic and hybrid active layers as well as film and device degradation. Since 2016, we also have a focus on device up-scaling through Roll-to-Roll (R2R) printing technology at the SDU R2R facility.
I have been supervisor of 11 PhD projects, 3 currently running, and 12 postdocs, of which 5 are currently running.
In total 83 publications: 63 peer-reviewed journal articles, 11 peer-reviewed conference proceedings, 2 books (editor), 4 book chapters, and 3 others. Includes publications in Nature, Nature Energy.



e-mail: kulda@ill.fr

Prof. emeritus Jiri Kulda
Institut Laue-Langevin
France

Dr. Jiri Kulda is leading scientist emeritus at the Institut Laue-Langevin (ILL), Grenoble. Since 1991 until his retirement at the end of 2017 he has been successively instrument scientist and group leader of the Tripple Axis Spectrometers. Before joinin the ILL he has spent some years as scientist and senior scientist at smaller neutron sources at the Nuclear Physics Institute at Rez near Prague (CR) and at the Laboratory of Neutron Physics, JINR, Dubna (USSR). All his degrees are in experimental solid state physics and come from the Czech Technical University in Prague (CR). His major scientific interests are on one hand scattering theory, neutron optics, design and construction of neutron instruments and on the other hand the use of neutron and Xray scatter-ing to study both static and dynamic correlations in disordered crystalline systems.



e-mail: zeynep.altintas@tu-berlin.de

Prof. Dr. Zeynep Altintas
Technische Universität Berlin
Germany

Zeynep Altintas is a full professor and the Chair of Bioinspired Materials and Biosensor Technologies at the University of Kiel, Germany. She has been the Head of Biosensors and Receptor Development Group at the Technical University of Berlin since 2016. She completed her Ph.D. on biomedical sensors at the age of 25 with the outstanding Ph.D. student award. Her Ph.D. period brought her several other research prizes and fellowships. Following a one-year post-doc position at the Cranfield Biotechnology Centre, she continued her academic career as a faculty member of Biomedical Engineering at Cranfield University (the UK) until 2016. She leads an interdisciplinary research group in the domains of biosensor technologies, computational chemistry, receptor design, functional polymers and their applications in (bio)chemical sciences, nanomaterials applications, and design, synthesis, and characterization of biomimetic materials. She has >170 publications in these fields, including books, journal articles, book chapters, patent applications, and conference papers. She has supervised more than 35 Ph.D. and M.Sc. students and mentored seven post-doctoral fellows.s



e-mail: tony.donne@euro-fusion.org

Prof. Tony Donné
EUROfusion
Germany

Tony Donné is since June 2014 Programme Manager (CEO) of EUROfusion; a consortium of 30 national research institutes and about 150 universities in 28 European countries. From 2009 – 2014 he coordinated the Dutch research activities in the field of fusion research. He was founding director of the Dutch-Russian Centre of Excellence for Fusion Physics and Technology and he was Programme Director of the ITER-NL consortium. Almost his complete scientific career he has worked in the field of plasma diagnostics at a great range of fusion devices. He was closely involved in the design and developments of diagnostics for ITER. In 2010 he was appointed Professor in Diagnostics and Heating of Fusion Plasmas at Eindhoven University of Technology, Netherlands. He is presently chair of the Coordinating Committee of the International Tokamak Physics Activity; a worldwide organisation that coordinates research in support of the ITER project.



e-mail: anja-verena.mudring@chem.au.dk

Prof. Dr. Anja-Verena Mudring
Department of Materials and Environmental Chemistry, Stockholm University
Sweden
Department of Chemistry, Aarhus University
Denmark

Anja-Verena Mudring studied chemistry at the Rheinische-Friedrich-Wilhelms Universität zu Bonn (D, 1990-1995) and carried out her Dr. rer. nat. thesis work at Max-Planck Institute for Solid State Research (D, 2001). Postdoctoral research took her to as a Feodor Lynen Fellow of the Alexander von Humboldt foundation to Iowa State University and the U.S. DOE Ames Laboratory (USA, 2001-2003). In 2003 she started her independent academic career at the Universität zu Köln supported by a Liebig fellowship. After completing her Habilitation (2006), she become professor for inorganic chemistry at the Ruhr-Universität Bochum (D). In 2014 she moved back to Iowa State University as the Glenn Murphy professor and became a faculty scientist at the newly founded Critical Materials Institute at the U.S. DOE Ames Laboratory (USA). In 2017 she moved to the Department of Materials and Environmental Chemistry at Stockholm University (SWE) where she established a program on Green Chemistry and, most recently, became founding director of the Stockholm University Center for Circular and Sustainable Systems (SUCeCSS). Her newest academic adventure is taking her as a Villum Investigator and iMAT professor to Aarhus University (DK) where she was also elected as an Associate Fellow of the AU Institute of Advanced Studies in 2021. Moreover, she is currently an Honorary Professor at the College of Engineering, University of KwaZulu-Natal, South Africa. Prof. Mudring is currently acting as editor-in-chief for the journals Green Chemistry Reviews & Letters and Polyhedron.

Her research motto is ¨Theory with Practice¨ and research in the Mudring group is driven by understanding fundamental structure-property relationships with the aim to design new materials for energy related applications for a sustainable society. Applications in focus are energy efficient lighting, (photo-)catalysis, magnetic refrigeration and thermoelectric energy conversion. All of which help, in a direct or indirect way, to meet the Sustainable Development Goals as being put forward in the United Nations Development Programme. In her materials development approach AVM takes a holistic approach: The materials should be benign by design, green in application and their manufacturing also should be environmentally benign. In this, she is using the principles of Green Chemistry & Engineering.

Her research has been supported by the major funding agencies such as the German Science Foundation, the US Department of Energy, the National Science Foundation, Vetenskapsrådet, the Knut and Alice Wallenberg, Villum, Novonordisk and Carlsberg Foundations.



e-mail: arunas.ramanavicius@chf.vu.lt

Prof. Dr. habil. Arunas Ramanavicius
Vilnius University
Lithuania

Prof. Habil. Dr. Arunas Ramanavicius is a professor at Vilnius University, Vilnius, Lithuania. He is also leading the laboratory of NanoBioTechnology at Research Center of Physical Sciences and Technologies. Prof. Arunas Ramanavicius is a member of Lithuanian Academy of sciences. In 1998 he received PhD degree and in 2002 doctor habilitus degree from Vilnius University. He has research interests in various aspects of nanotechnology, bionanotechnology, nanomaterials, biosensorics, bioelectronics, biofuel cells and MEMS based analytical devices. He was a national coordinator of several nanotechnology related COST actions. Editorial board member of Materials; Sensors; Chemija and several other journals.
Prof. A. Ramanavicius is serving as expert-evaluator in Horizon 2020 program coordinated by European Commission and he is technical advisor of many foundations located in European and non-European countries.



e-mail: simas.rackauskas@ktu.lt

Dr. Simas Rackauskas
Kaunas University of Technology, Institute of Materials Science
Lithuania

Simas Rackauskas is a Chief Researcher in Kaunas University of Technology (KTU). He defended his PhD in Physics at Aalto University, Finland in 2011. He was a Marie Curie Fellow in University of Turin (Italy). He had fellowships in Swiss Federal Institute of Technology in Lausanne (EPFL, Switzerland), Technical University of Denmark (DTU) and University of Nagoya (Japan). His research interests are mainly focused on non-catalytic growth mechanisms of metal oxide nanowires and application in sensing and multifunctional coatings. He is involved in commercialization in anti-reflection coatings in spin-off "Zinotech" (CEO).



e-mail: angela.ivask@ut.ee

Prof. Dr. Angela Ivask
University of Tartu, Institute of Molecular and Cell Biology
Estonia

Angela Ivask is Professor at the University of Tartu Institute of Molecular and Cell Biology. She has graduated from Tallinn University of Technology as molecular biologist. Since 2007 she has been involved in nanomaterial-related research, mainly from the point of view of biological effects of such materials. During her post-doctoral training at the Center of Environmental Implications of Nanotechnology of UCLA and at the Future Industries Institute of the University of South Australia , A. Ivask studied the mechanisms of action of nanomaterials on bacteria and human cells. Since 2015 the focus of her research has been innovative applications of nanomaterials and with collaboration of the Institute of Physics of the University of Tartu, she has developed nanomaterial-based coatings for antimicrobial use. Currently she is leading a research group on microbe-material interactions and her studies focus on one side, on the development of industrially feasible rapidly acting antimicrobial coatings and on the other hand, on microbial stress responses induced upon antimicrobial treatments.



e-mail: mikhael.bechelany@umontpellier.fr

Dr. Mikhael Bechelany
Institut Européen des Membranes
France

Mikhael Bechelany (born in March 1979) obtained his PhD in Materials Chemistry from the University of Lyon (France) in 2006. His PhD work was devoted to the synthesis and characterization of silicon and boron based 1D nanostructures (nanotubes, nanowires and nanocables). Then, he worked as a post-doc at EMPA (Switzerland). His research included the fabrication of nanomaterials (nanoparticles and nanowires), their organization and their nanomanipulation for applications in different field such as photovoltaic, robotic, chemical and bio-sensing. In 2010, he became a Scientist at CNRS. His current research interest in the European Institute of Membranes (UMR CNRS 5635) in Montpellier (France) focuses on novel synthesis methods for metals and ceramics nanomaterials like Atomic Layer Deposition (ALD), electrodeposition, electrospinning, 3D printing and/or on the nanostructuring using natural lithography (nanospheres and/or membranes). His research efforts include the design of nanostructured membranes for health, environment and renewable energy. Beginig of 2022, he is the author and co-author of more than 280 publications, 13 book chapters and 10 patents (h-index = 55). He is also the co-founder of 3 Startups.



e-mail: samuel.lara@chalmers.se

Assist. prof. Samuel Lara Avila
Chalmers University of Technology
Sweden

"Graphene might be the only known material that remains an excellent conductor of electricity/heat even when having, effectively, no electrons. We have reached a near zero-electron scenario in graphene, also called Dirac point, by assembling electron-accepting molecules on its surface. Our results show that graphene is an exceptionally good material for THz heterodyne detection when doped to the Dirac point", says Samuel Lara-Avila, assistant professor at the Quantum Device Physics Laboratory.



e-mail: coyeme@amu.edu.pl

Assoc. prof. Emerson Coy
NanoBioMedical Centre, Adam Mickiewicz University
Poland

Emerson Coy is an associate professor at the NanoBioMedical Centre of Adam Mickiewicz University, Poznań, Poland. He received his Habilitation degree in material sciences from the AGH University of Science and Technology, Poland, in 2019. He received his PhD degree in nanoscience from the University of Barcelona, Spain, in 2016, his master's degree in applied and computational physics from the Polytechnic University of Catalonia, Spain, in 2009, and his master's degree in nanotechnology from the University of Barcelona in 2008. Additionally, Coy holds an engineering degree from Manuela Beltran University, Colombia, obtained in 2006. His research interests include thin films/coatings, multiferroics, carbides, nanoindentation, composite materials, photoelectrocatalysis and energy harvesting.



e-mail: sergei.vlassov@ut.ee

Assoc. prof. Sergei Valssov
Institute of Physics, University of Tartu
Estonia

Sergei Vlassov is an associate professor and the leader of the nanomanipulation team at the Institute of Physics, University of Tartu. Sergei has a Ph.D. in Material Science (2011, University of Tartu) and a Master's Degree in Applied Physics (2007, University of Tartu). His research activities are focused mainly on experimental investigations of various nanostructures and nanostructured materials for functional applications and future technologies. At the moment Sergei is responsible for the nanotechnology-related field in EraChair "MATTER" project in Estonia.



e-mail: kestutis.staliunas@icrea.cat

Prof. Kestutis Staliunas
Universitat Politecnica de Catalunya
Spain
Vilnius University
Lithuania

K. Staliunas is ICREA (Institució Catalana de Recerca i Estudis Avançats) professor in Department of Physics of Universitat Politecnica de Catalunya (UPC), Barcelona, head of research group on lasers, micro-lasers, photonic and sonic systems, non-Hermitian systems, nonlinear optical patterns. He is author of more than 200 articles with more than 7000 citations (h-factor 48), more than 500 presentations in conferences. His research interests are: pattern formation in lasers, microlasers, metamaterials and metamirrors, in non-Hermitian spatially extended systems. Since 2020 he is also State Professor in Vilnius University (VU). Up to now directed (or currently directed) 20 PhD projects.



e-mail: jose.montero-amenedo@angstrom.uu.se

Dr. José Montero Amenedo
Division of Solid State Physics, The Ångström Laboratory, Uppsala University
Sweden

José Montero Amenedo holds a BSc + MSc in Physics from Salamanca University (Spain) and a MSc + PhD in Physics from CIEMAT/Complutense University of Madrid (Spain). Since 2018, J.M. is a Researcher within Prof. Lars Österlund's Group at the Division of Solid State Physics, The Ångström Laboratory, Uppsala University.
J.M.'s research interest comprises transparent conducting oxides, photocatalytic materials and chromogenic materials (electrochromic, thermochromic and photochromic), among others. Generally speaking, J.M.'s research efforts can be contemplated from a green-nanotechnology perspective, i.e., the use of nanotechnology for minimizing the impact of human activity on the environment.



e-mail: Simon.Woodward@nottingham.ac.uk

Prof. Simon Woodward
University of Nottingham
United Kingdom

Simon Woodward is a Professor of Synthetic Organic Chemistry at the University of Nottingham (UK) since 2006. Prior to that he held a lectureship at the University of Hull (UK) and postdoctoral positions at the Universities of Oxford (UK) and Michigan (USA), the latter as a Fulbright Scholar. Simon Woodward's background is in developing efficient, often catalytic, syntheses of small organic molecules and in attaining understanding the reaction mechanisms by which such products are formed. However, for more than the last decade he has been interested in the preparation of new and existing organic electronic molecular building blocks for application in thermoelectric (TE) devices. Our current work at the GSK Carbon Neutral Laboratory emphasises the attainment of these targets by methods that minimise waste and maximise safety/utility. My co-researchers and I have popularised the use of the air stable trimethylaluminium analogue DABAL-Me3, but have also commercialised other reagents and organic materials including some aromatics, an area we are presently seeking to expand into new areas.



e-mail: klassen@hsu-hh.de

Prof. Dr. Thomas Klassen
Institute for Hydrogen Technology at Helmholtz-Centre, Hereon Institute of Materials
Technology at Helmut Schmidt University
Germany

Thomas Klassen holds a shared professorship as director of the Institute for Hydrogen Technology at Helmholtz-Centre Hereon in Geesthacht, and as head of the Institute of Materials Technology at Helmut Schmidt University / University of the Federal Armed Forces Hamburg, Germany. His Ph.D. research and 2-year post-doc stay at the University of Illinois at Urbana-Champaign related to basic mechanisms during production of nanocrystalline materials as well as their particular properties and potential applications. His current research focus at the Institute for Materials Technology at Helmholtz-Zentrum Geesthacht lies on green hydrogen generation and storage technology. At Helmut-Schmidt-University, research concentrates on kinetic spraying of particles with sizes in the nano and micrometer range as novel coating technology, from powder design to tailored functional properties and applications. Thomas Klassen is one of the pioneers in the field of nanocrystalline materials for hydrogen technology, including reactive hydride composites. He published more than 250 papers (with over 10k citations, h-factor 45) and more than 20 patents, presented 80 invited and keynote presentations, and is co-founder of the company KSS-Kinetic Spray Solutions GmbH.



e-mail: romanas.zontovicius@kaunomtp.lt

Romanas Zontovičius
Kaunas Science & Technology Park
Lithuania

Romanas Zontovičius is a Director of Innovation and Entrepreneurship Development Department at Kaunas Science and Technology Park. Before joining the Park Romanas worked for various IT companies in Silicon Valley (San Francisco Bay Area, USA). 7 years with GetJar, one the most successful Lithuanian startups. He did Sales and Sales Operations and was a primary contact for many key clients such as Facebook, Google, Amazon, Zynga, eBay, and many others. When at Spigot he was VP of Sales and managed major deals with foreign telecoms. When at Nextury Ventures he mentored portfolio startups, help them get into various acceleration programs, and was their agent in Silicon Valley. For the last 2 years Romanas worked with Waymo/Goggle, the creators of autonomous vehicles as a lecturer/senior instructor who taught classes for the current and future safety drivers as well as future safety instructors. Currently Romanas runs a Startup pre-accelerator called Evolut 4.0 at Kaunas STP.



e-mail: Marco.Kirm@ut.ee

Prof. Marco Kirm
University of Tartu
Estonia

Marco Kirm, born in 27.12.1965, is a professor of experimental physics at the University of Tartu. He graduated cum laude as a physicist from University of Tartu in 1991 and obtained his PhD „Spectroscopy of highly charged ions, small molecules and solids under VUV excitation", supervised by Prof. Indrek Martinson, at Lund University in 1995. During 1997-2004 he worked at Hamburg University in the group of Prof. Georg Zimmerer as a post-doctoral researcher. Being in duties of a beam-line scientist he was responsible for operation of the famous SUPERLUMI station (HASYLAB, DESY), which served luminescence community at highest level for many years. Since 2004 after return to Estonia, he has been in duties of a research director and director of the Institute of Physics of the University of Tartu. During 2012-2017 he was appointed as a Vice Rector for Research of the University of Tartu. In 2012 Marco Kirm was elected to the Latvian Academy of Sciences as a foreign member and in 2018 as a member of Estonian Academy of Sciences. He is also a member of the International Advisory Board of Institute of Solid State Physics at Latvian University in Riga. Internationally he serves as an Estonian member of the Euratom Scientific and Technical Committee. Nationally he acts as a chairman of the councils in of the Estonian roadmap objects of research infrastructures: NAMUR+ (Centre of Nanomaterials Technologies and Research) and FINESTBEAMS (Estonian Beamline at MAX-IV Synchrotron Radiation Source). He is also active in coordinating Estonian research activities within Crystal Clear Collaboration at CERN.

His research interests cover wide range of novel functional wide gap materials (incl. nano-materials) applicable as LED phosphors, scintillators. He is also carrying out research on basic phenomena such as relaxation processes of electronic excitations and their dynamics by luminescence spectroscopy in wide time, temperature and energy range; ultrafast radiative processes (applications in PET tomography); creation of radiation defects in wide gap solids. He also focuses on novel optical diagnostics methods for thin dielectric films and optical materials. He is a spokesperson of Estonian-Finish beamline FinEstBeAMS at the MAX IV Lab in Lund, Sweden. His publication list includes 268 papers, cited over 4000 times as found in the WoS. In order to fulfil his research goals, he is regularly using advanced light sources in large scale research centres: DESY in Germany (PETRA III, FLASH), MAX IV Lab in Sweden (FinEstBeAMS, FemtoMAX) and at the laboratories of LASERLAB-EUROPE (VULRC in Lithuania, LIDYL in France).

In European Research Area he served as a long term representative (2006-2014) of Estonia at the COST (Cooperation in Science and Technology, EU) in "Materials science, physics and nanosciences" domain committee. The INTERREG Baltic Sea Region innovation projects "Science Link" (2011-2014), "Baltic Tram" (2016-2019) and "Carots" (2019-2021) with a focus on industry academia cooperation are governed by him in Estonia.

Marco Kirm's continuously updated complete CV (incl. publications, research projects, etc.) can be found at the Estonian Research Portal.



e-mail: pucker@fbk.eu

Dr. Georg Pucker
Fondazione Bruno Kessler, Center for Materials and Microsystems
Italy

Dr. Georg Pucker is the head of the Advanced Materials and Photonic Structures research unit within the Center of Materials and Microsystems, Fondazione Bruno Kessler, Trento. He obtained his Doctoral degree in Technical Chemistry from the Technical University in Graz in 1996. Since 2001, he is researcher at the Center for Materials and Microsystems of FBK. His research in FBK ranges from silicon radiation detectors, solar cells, heterointegration of materials to silicon platforms and to integrated silicon photonics. The research in silicon photonic foccuses on the realisation of optical circuits and on the study of non-linear optical properties of silicon and silicon compatible materials. He has contributed to several projects of the European community, namely Esprit Project 28741 – SMILE (Silicon Modules for Integrated Light Engineering); Nemo (Nano based capsule Endoscopy with molecular imaging and optical biopsy) FP6-37362 STREP; FP6-37026 Anna (European Integrated Activity of Excellence and Networking for Nano and Micro- Electronics Analysis FP6-37026, and FP7- Symphony (Integrated SYsteM based on PHOtonic Microresonators and Microfluidic Components) and was the principal investigator of FBK for the project LIMA (Improve Photovoltaic efficiency by applying novel effects at the limits of light to matter interaction, FP7-248909). Currently, he is the principal investigator of FBK of the project Siquro (On silicon chip quantum optics for quantum computing and secure communications) financed by the Autonomous Province of Trento. He is author or co-author of more than 80 peer reviewed publications, author of a book chapter and inventor of 3 patents.



e-mail: juras.banys@ff.vu.lt

Prof. Dr. habil. Jūras Banys
Faculty of Physics, Vilnius University
Lithuania

Prof. Jūras Banys is Doctor habilis (Physical Sciences), professor, academician at the Lithuanian Academy of Sciences.
From 1989 to 1990 he worked at the University of Oxford (UK) with a grant from Georges Soros Foundation.
Having received Alexander von Humboldt Foundation Scholarship, from 1993 to 1995 Banys worked at the University of Leipzig, Germany.
In 2000, he was awarded the Povilas Brazdžiūnas Prize of the Lithuanian Academy of Sciences. In 2002, Banys was awarded the Lithuanian Science Prize.
In 2011, Jūras Banys was elected full member of the Lithuanian Academy of Sciences.
Main research areas:
Lattice dynamics, ferroelectricity, structural phase transitions, dipolar glasses, relaxors, dielectric spectroscopy, multiferroics, composites, EPR
Membership in organisations:
Foreign member, Latvian Academy of Sciences
Corresponding member, Saxon Academy of Sciences, Germany
Member of the Board, Lithuanian Physical Society
Member of the Editorial Board, Lithuanian Journal of Physics
European Conference on Applications of Polar Dielectrics, member of the International Advisory Board
European Committee on Ferroelectricity
International Committee of Electroceramics, member
Ferroelectrics Standing Committee of the IEEE Ultrasonics, Ferroelectrics, and Frequency Control Society, member
AMPERE Society Committee
Honorary Degree of Uzhhorod National University



e-mail: andreas.scherz@xfel.eu

Dr. Andreas Scherz
European XFEL GmbH
Germany

Dr. Andreas Scherz is leading scientist and group leader of the Spectroscopy and Coherent Scattering (SCS) Instrument at the European XFEL since 2012. Before, he joined the SLAC National Accelerator Center as a Postdoc in 2004 and became later a staff scientist at the Stanford Institute for Material and Energy Science (SIMES). His major research interest are ultrafast magnetism and laser-driven phase transitions in quantum materials on nanometer length scales and advancing X-ray methodologies such as time-resolved spectroscopies and holographic imaging in the soft X-ray region.



e-mail: shku@mci.sdu.dk

Assoc. prof. Shailesh Kumar
Centre for Nano Optics, University of Southern Denmark
Denmark

Shailesh Kumar is an assistant professor at the Centre for Nano Optics, University of Southern Denmark. He obtained his Ph.D. degree in Physics from the Technical University of Denmark (DTU), Denmark in 2012. His area of research includes light-matter interaction, quantum plasmonics, and integrated quantum optics. He has mainly worked on enhancing the emission properties of quantum emitters by coupling them to various nanostructures, such as nanocavities, plasmonic waveguides, and meta-surfaces.



e-mail: Gunta.Kunakova@lu.lv

Dr. Gunta Kunakova
Institute of Chemical Physics, University of Latvia
Latvia

Dr Gunta Kunakova is senior researcher at the University of Latvia, Institute of Chemical Physics. Her research currently focuses on exploring exotic phases of matter in 2D hybrid materials and nanostructured topological insulators.
She defended her PhD thesis in Chemistry, at University of Latvia in 2015 and thereafter joined as a postdoc prof. F. Lombardi's group at Chalmers University of Technology, Sweden (SI scholarship and PostDoc Latvia grant).



e-mail: raivo.jaaniso@ut.ee

Dr. Raivo Jaaniso
Laboratory of sensor technologies, University of Tartu
Estonia

Dr Raivo Jaaniso is the head of the laboratory of sensor technologies at the University of Tartu. During his career, he has worked in various solid-state and applied physics areas. He obtained his PhD from the Institute of Physics at the Estonian Academy of Sciences and thereafter worked as a postdoc at the University of Geneva. His interests were in laser spectroscopy and spectral hole burning of the impurity solids. At the University of Tartu, he initiated a new applied research direction, concentrating on developing luminescent and semiconductor gas sensor materials and physical models of the processes involved. Currently, his interests are focused on designing novel sensing (hetero)structures based on graphene and related nanomaterials and new signal read-out and processing methods for applications involving multi-response sensors or sensor arrays.



e-mail: m.hoedl@fkf.mpg.de

Dr. Maximilian F. Hoedl
Max-Planck Institute for Solid State Research
Germany

Maximilian Hoedl is a post-doctoral researcher at the Max-Planck Institute for Solid State Research in the group of Prof. Joachim Maier. His research focuses on mixed electronic-ionic conducting materials that are particularly useful for fuel-and electrolyzer cells. In 2021 he received his PhD in the same group where he studied the interactions between electronic and ionic charge carriers in iron-containing perovskite oxides. Currently, he is continuing his research on these materials by studying the mobility of ionic defects.



e-mail: Jevgenijs.Kotomins@cfi.lu.lv

Dr. habil. Eugene Kotomin
Institute of Solid State Physics, University of Latvia
Latvia

Dr. habil. phys., PhD, Eugene Kotomin (Jevgenijs Kotomins) is senior scientist in the Laboratory of Self-organizing Systems, Institute of Solid State Physics, University of Latvia, Riga.
Full member of Latvian Academy of Sciences, Citation H-index: 51 (WoS), total citations 10.000+, 520+ papers in refereed journals, 17 books and book chapters, 12 review articles. Main research interests include: Theoretical materials science based on first principles calculations. Theory of radiation-induced effects and defects in solids, kinetics of reactions with a focus on self-organization phenomena in diffusion-controlled reactions, Quantum chemistry of defective solids, nanomaterials and surfaces/interfaces.



e-mail: asta.tamuleviciene@ktu.lt

Assoc. prof. Dr. Asta Tamulevičienė
Institute of Materials Science, Kaunas University of Technology
Lithuania

Dr Asta Tamulevičienė is currently a senior researcher and part time associate professor at the Kaunas University of Technology (KTU). Her research through all the carrier was related to the light phenomena, either via the analysis of optical properties of the materials or application of light-based analytical methods to determine the structure of the materials. She is a member of the KTU research group Applied Optics and Photonics. She has experience in vacuum film deposition and characterization of diamond like carbon nanocomposite films (PhD thesis defended in 2012). Currently her interests are the synthesis of noble metal nanoparticles and application of nanoparticles for the sensors based on Surface Enhanced Raman Scattering (SERS).



e-mail: ssch@tf.uni-kiel.de

Ph.D. Stefan Schröder
Kiel University
Germany

Stefan Schröder pursued his Ph.D. studies on initiated chemical vapor deposition of new electronic and multifunctional polymer thin films at Kiel University, Germany under the supervision of Prof. Faupel including a research stay in Prof. Gleason's group.
After finishing his Ph.D. in 2021, he then continued as a subgroup leader for functional CVD Polymers at the Chair for Multicomponent Materials (Prof. Faupel) in Kiel.
His research interest include chemical vapor depostion, polymer thin films and theoretical approaches for electronic structure calculations.



e-mail: egidijus.urbonavicius@lei.lt

Dr. Egidijus Urbonavicius
Lithuanian Energy Institute
Lithuania

Egidijus Urbonavičius graduated Vytautas Magnus University as Master of Science in Physics in 1998. In 1995 during bachelor studies in university he started professional career at Lithuanian Energy Institute (LEI) in Ignalina Safety Analysis Group, which later became Laboratory of Nuclear Installations Safety. In 1998 he started PhD studies at LEI and in 2003 he successfully defended Doctor theses in the field of thermal engineering and continued professional career at LEI. At LEI he grew from assistant in laboratory to chief researcher.
The main topics of interest in science are processes in containments on nuclear power plants in case of severe accidents covering entire spectrum from thermal-hydraulics to transport of the radioactive fission products and definition of source term to environment. In 2006 he also became involved in research linked with the fusion facilities and was a leader of first fusion project liked with safety assessment of ITER facility in the frames of EURATOM in Framework Program (FP-6). After LEI joined implementation of European Fusion Development Agreement (EFDA) in 2007 he became the main contact point with European Commission for project implementation. In 2015 he was a deputy project leader for the first H2020 project coordinated by LEI. In 2019 he became a Head of Research Unit of LEI for implementation of EUROfusion project.
He is an author of more than 50 scientific publications, including 1 monograph on Severe accident management for Ignalina NPP.



e-mail: Anatolijs.Popovs@cfi.lu.lv

Dr. Anatoli I. Popov
Institute of Solid State Physics University of Latvia
Latvia

Anatoli Popov is a senior research fellow at the Institute of Solid State Physics of the University of Latvia. In 1984 he graduated from the Moscow Institute of Physics and Technology, and in 1990 he defended his Ph.D. thesis at the Institute of Physics of the Latvian Academy of Sciences. According to SCOPUS, he is the co-author of over 230 articles with over 3400 citations and an H=35 index. He has been the Principal Investigator in several projects funded by the Latvian & European Research Program (EUROfusion) totaling around 1.5 million euros. He has worked as a visiting scientist at the Kernforschungzentrum Juelich GmbH (Germany) and the French National Research Center for Nuclear Physics (GANIL). He then was a visiting professor at the Carlos III University of Madrid (Spain) and a staff scientist at RIKEN, Japan. From 2000 to 2010 he was in Grenoble as a researcher at the European Molecular Laboratory and the Laue-Langevin Institute. His main research interests include the experimental and theoretical study of electronic and optical properties of solids, radiation effects and defects in solids, radiation detection, applications of neutron, swift-heavy ion and synchrotron radiation in solid state research. He is a member of Fusion Science Department Project Board and also member of the Board on Materials in EUROfusion enabling research programme. He is also a board member of Crystal Clear Collaboration at CERN and visiting professor of Eurasian National University in Kazakhstan. In addition, in 2021 and 2022, he is the main organizer of two EMRS symposiums on the topic “Defects in Nanomaterials”, and in 2024 he will be the host of the International Conference on Luminescent Detectors and Transformers of Ionizing Radiation, which will be held in Riga in 2024



e-mail: sergii.b.ubizskii@lpnu.ua

Prof. Sergii Ubizskii
Lviv Polytechnic National University
Ukraine

Sergii Ubizskii, Dr.Sc., Prof., Professor at the Department of the Semiconductor Electronics, Lviv Polytechnic National University. Has graduated (1983) from Physical Department of the Ivan Franko National University of Lviv (Ukraine), got degree of Cand.Sc. (1991) from the same university and degree of Dr.Sc. (2001) from Lviv Polytechnic National University. Worked in Scientific Research Company "Electron-Carat" (1983-1997) and since 1997 works in Lviv Polytechnic National University. Has got a title of Professor in 2005. Main research activity is related to investigation of mainly optical and magnetic properties of oxides and related materials in the form of single crystals, crystalline films, ceramics, nanoparticles and composites, their fabrication technology and after-synthesis modification by means of thermo-chemical treatment and irradiation, as well as their usage in devices of quantum- and optoelectronics, sensors of radiation, magnetic field etc., other transducers and convertor devices including biomedical applications. Has published more than 140 papers in peer reviewed journals, in particular more than 50 in the journals of quartiles Q1 and Q2, as well as 2 monographs, 2 textbooks, 11 patents. Since 2007 has organized 6 International Scientific Conferences on Oxide Materials for Electronic Engineering – Fabrication, Properties and Application (OMEE), the last of which held in 2021.



e-mail: Kaspars.Traskovskis@rtu.lv

Assoc. prof. Kaspars Traskovskis
Riga Technical University
Latvia

Kaspars Traskovskis is an associate professor at Riga Technical University (RTU), Faculty of Materials Science and Applied Chemistry. In 2014 he received his PhD degree in organic chemistry at RTU. His thesis was devoted to the development of organic molecular glass-forming materials with optoelectronic functionality. His current work is focused on synthesis and investigation of novel light-emitting organometallic compounds for use in cost-efficient organic light emitting diodes (OLEDs).

ABSTRACTS

of the **PLENARY PRESENTATIONS**

Azobenzenes and Diazocines for Light Switchable Materials

Anne Staubitz
University of Bremen

Azobenzenes, be it in a linear arrangement or in rings, are important molecular switches that can change their geometry by the absorption of light of specific wavelengths. Although this is well-established, the demands of biologists and materials scientists for very specific requirements in terms of switching wavelengths, half-live times and chemical functionality have increased steeply. Synthetic chemists often find that if one strays beyond the well-known and established, there are no synthetic routes available, which must be newly invented. As a consequence, with such methods available, new, exciting and often unexpected materials developments can take place.

This presentation will present new synthetic methodology that was recently invented in our laboratories. In addition, new materials that arise from these azobenzenes and diazocines will be shown: The liquid crystals were analysed by DSC and POM and their photomechanical effect was demonstrated visually.

A new design principle was developed that allowed to confer liquid crystallinity to azobenzene based switching liquid crystals that bend with visible light.

We have now a material available that can be used in the area of soft robotics.

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Development of promising nanostructured thermoelectric materials and their hybrids through sustainable chemical routes

Muhammet S. Toprak
KTH Royal Institute of Technology

Thermoelectric (TE) materials are capable of converting waste-heat to electrical energy. They can have a big impact on sustainable transition, if its large-area applications can be realized. This is limited due to the inherent limitations of materials stability, or the cost of materials and their production.

Nanostructured TEs, are normally fabricated using a bulk process rather than a nano-fabrication process, which has the important advantage of producing in large quantities and in a form that is compatible with commercially available TE devices.

We developed and demonstrated colloidal fabrication of some well-known TE materials as $FeSb_2$, Bi_2Te_3, Sb_2Te_3, $Bi_{2-x}Sb_xTe_3$, and $Cu_{2-x}Se$ as nanostructures. in a matter of minutes using MW-assisted heating. We repeatedly demonstrated improvements in the TE performance of various materials, by designing high-throughput, scalable, energy effective synthetic methodologies resulting in well-defined nanostructured building blocks. The focus was first on the Bi-Sb-Te materials (n- and p-type), which was then applied to p-type and earth abundant compositions including Cu_2Se, Cu_2S, $CuFeS_2$.

Our research shows the significance of the preparation route on the resultant material's morphology, particle size, microstructure and transport properties. Our preliminary studies showed a successful intercalation of synthesized Sb-telluride and Bi-telluride nanoparticles into a PMMA matrix, during which we identified some key process parameters and interface modifiers (or performance boosters), causing strong influence on the charge transport between the two phases, reaching impressive power factor.

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ORGANIC PHOTOVOLTAICS: FROM THIN FILM SYNTHESIS TO LARGE SCALE MANUFACTURING

Morten Madsen

University of Southern Denmark, Mads Clausen Institute

Organic photovoltaic (OPV) devices have recently experienced a fast rise in power conversion efficiency (PCE) with the introduction of new non-fullerene acceptor (NFA) molecules, reaching today PCE values above 18 %, placing device stability and large-scale manufacturing as the focus areas for this technology. In this presentation, recent progress on active layer molecule and interlayer systems as well as device architecture and up-scaling routes will be presented. Transition metal oxides have been demonstrated as an important class of materials for OPV devices, where they serve as charge carrier selective interlayers for efficient electron and hole extraction. However, interlayer related instabilities have recently been reported as a main degradation route for NFA OPV devices, making a thorough understanding of such interface effects highly important for the further development of this field and technology. Recent progress made within sputtered metal oxide electron [1,2] and hole [3] transport interlayers for thin film organic photovoltaics will be presented. Supported by a variety of surface science characterization techniques, the role of e.g. microstructure, work function, oxygen vacancies and energy band alignment, on the performance of such interlayers in organic photovoltaic devices is discussed. This includes a focus on their positive impact on non-fullerene acceptor based OPV device stability, as compared to conventional metal oxide interlayers. Here, new results focusing on the integration of 2D materials in NFA OPV will also be elaborated on.

In addition, routes for Roll-to-Roll (R2R) up-scaling and manufacturing of OPV will be presented, including metal oxide interlayers and full modules using industrial-compatible techniques. This includes (R2R) UV Nanoimprint Lithography (UV NIL) for improving the light absorption in fully scalable OPV. Nanoscale structures are formed on flexible substrates using R2R UV nanoimprint lithography and integrated in fully scalable OPV devices to form efficiency-enhanced ITO-free OPV [4]. The nanostructured OPV are based on the non-fullerene acceptor system PBDB-T: ITIC, and made in a back contact nanostructured grating architecture. All the processes are made in an ambient condition from non-toxic solvents, and can easily be adapted to the industrial standard. Using optical modelling, the effect of the nanostructured grating on the performance of OPV devices is investigated and optimized. Due to combined effects of improved charge carrier extraction and enhanced optical path lengths, these industrial compatible nanostructured OPV reach device power conversion efficiency enhancements of above 20%.

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From molecular dynamics simulations to diffuse scattering maps

Jiri Kulda
Institut Laue-Langevin

Modern materials often exhibit a considerable portion of structural disorder, playing a key role in their functionalities. In order to characterise local atomic arrangements and short-range correlations one has to study the shape of Bragg lines and the distribution of diffuse scattering below and between them.

To extract information from experimental data one has to compare model-based intensities with the observed ones. The progress in computing techniques in last decades permits to produce realistic models of crystalline lattices by a variety of approaches ranging from ab initio DFT methods via molecular dynamics (MD) to phase-field models based on the Landau formalism. Alternatively, one may retrieve the displacement pattern without making assumptions on its origin by reverse Monte-Carlo (RMC) modelling

With this progress in place the bottleneck has shifted from producing supercell models to generating the corresponding diffuse scattering distributions in reciprocal space. The principal issue being the fact that scattering amplitudes from a distorted lattice cannot be summed up using fast Fourier transform algorithms (FFT) because of the displacement phase factor exp(-iQR) being Q-dependent. As a consequence, many efforts in recent years have been restricted to simple models on small supercells [1,2] or to more involved pair distribution function (PDF) analysis [3-5], where the summation problem is reduced to a single dimension.

To address this issue, we will present the results of a new approach [6], based on recent developments of the non-uniform fast Fourier transform algorithm [7], implemented in the MP_tools program suite [8]. Diffracted intensities from model supercells containing millions of atoms as well as dynamic scattering functions S(Q,ω) based on time sequences of thousands of frames can be addressed in an interactive manner.

Many motivating discussions with my colleagues Marek Pasciak, Petr Ondrejkovic and Jirka Hlinka from the Institute of Physics (AS CR) are kindly acknowledged.

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Biosensor applications of functional polymers

Zeynep Altintas

Technical University of Berlin, Strasse des 17. Juni 124, 10623 Berlin, Germany

The conformation of biological molecules on surfaces or in solution environments strongly effects the successful implementation of biosensing platforms for the detection of target molecules as possible conformational changes lead to decreased sensing signals. To date, artificial protein binders have been developed using linear peptides with an unknown structure in epitope imprinting process. Despite successful outcomes obtained to some extent, most of these works lack of providing either high affinity, selectivity or sensitivity.

We aim to address these problems by performing molecular dynamic calculations for the design of high affinity artificial protein binding surfaces for cancer biomarker recognition [1]. Computational simulations are employed to identify particularly stabile secondary structure elements. These epitopes are used for subsequent molecular imprinting, where surface imprinting approach is applied to obtain functional materials. The molecular imprints generated with the calculated epitopes of greater stability show better binding properties than those of lower stability. The average binding strength of imprints created with stabile epitopes is found to be around fourfold higher for the selected biomarker models [1]. The artificial protein binders can recognize the target molecules even in a complex medium including non-specific molecules at a high concentration [1-4]. Moreover, certain amino acid modifications of the computationally selected epitope templates (e.g. addition of histidine to the peptide chain or cysteine modification on both terminal of the elongated peptide to form self-assembled monolayer bridges) further improve the performance of artificial protein binders in biosensor applications [2-4].

Our novel and rational selection can be used for establishing epitope-based molecularly imprinted polymer (MIP) sensors for protein molecules by eliminating unsuitable epitopes and ranking the best candidates based on their stability analysis obtained from molecular dynamic simulations [1-4]. The integrated approach has shown a good potential to contribute to some limitations of medical diagnostic field. Research disciplines that require recognition receptors can apply this technique for designing stable and efficient receptors.

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Why don't we have fusion yet?

Tony Donné

EURO*fusion*, Garching, Boltzmannstr. 2, Germany

'Nuclear Fusion: an eternal promise' or 'Nuclear Fusion, always 30 years away' are texts one can read regularly in newspapers and journals. For the layman it is difficult put a finger behind the progress in the field of fusion research. This is especially because, after many years of research, still not even a milliwatt of electricity has been delivered to the grid. But are the abovementioned slogans correct?

Since the start of fusion research many different challenges had to be overcome. For example: how can a plasma (i.e. an ionized gas) be confined at temperatures that are 10 times higher than in the centre of the sun and how can we isolate this hot plasma from the walls of the reactor vessel, such that they will not melt. Many of the original challenges have been overcome in the global fusion research. But still much research needs to be done to tackle the remaining challenges. To prioritize the research in Europe, a Fusion Roadmap was developed with the international fusion reactor ITER, the demonstration reactor (DEMO) and the International Fusion Materials Irradiation Facility (IFMIF) as main research facilities. The Fusion Roadmap gives a reasonable indication how much more time is needed to get electricity from fusion.

The presentation will first shortly focus on the principle of nuclear fusion and magnetic confinement and the status of the field. An overview of the remaining challenges will be presented, along with a strategy to find adequate solutions:

1. **Plasma regimes of operation**: Demonstrate plasma that increase the success margin of ITER and satisfy the requirements of DEMO.
2. **Heat-exhaust systems**: Demonstrate an integrated approach that can handle the large power leaving ITER and DEMO plasmas.
3. **Neutron tolerant materials**: Develop materials that withstand the large 14MeV neutron flux for long periods while retaining adequate physical properties.
4. **Tritium self-sufficiency**: Find an effective technological solution for the breeding blanket, which also drives the generators.
5. Implementation of the **intrinsic safety features of fusion**: Ensure safety is integral to the design of DEMO using the experience gained with ITER.
6. **Integrated DEMO design** and system development: Bring together the plasma and all the systems coherently, resolving issues by targeted R&D activities
7. **Competitive cost of electricity**: Ensure the economic potential of fusion by minimising the DEMO capital and lifetime costs and developing long-term technologies to further reduce power plant costs.
8. **Stellarator**: Bring the stellarator line to maturity to determine the feasibility of a stellarator power plant.

ABSTRACTS

of the INVITED PRESENTATIONS

New and Improved Materials for Energy Applications Enabled by Ionic Liquids and Deep Eutectics

Anja-Verena Mudring

Department of Materials and Environmental Chemistry, Stockholm University, Svante Arrhenius vaeg 16c, 10691 Stockholm, Sweden

Nanomaterials have become indispensable for modern life. Many technologies depend critically on nanomaterials with engineered properties and structures, particularly those related to clean energy applications such as photocatalysts, light phosphors, thermoelectrics and others. Technological borders could be pushed further and improved materials would become available if more powerful tools for the tailored synthesis of nanomaterials could become available. In this, ionic liquids (ILs, room temperature molten salts) and deep eutectic solvents (DES) have the potential to become a true game changer. These unconventional solvents are permitting more efficient, safer and environmentally benign preparation of high quality products.

ILs, which can be built by a wide variety of cation-anion combinations with different functionalities, can act as the reaction medium, particle stabilizing and templating agent all-in-one, sometimes even as the reaction partner. IL based nanomaterial synthesis is faster, safer, and more energy- and atom-efficient than comparable methods. It uses less toxic chemicals, omits the use of auxiliary substances such as stabilizers, and minimizes waste. Through coupling with unconventional synthetic routes (physical vapor deposition, microwaves, ultrasound) that take advantage of their unique properties, ILs become even more powerful in nanomaterials synthesis.

Mixed systems such as DES offer a similarly broad combinatorial playground, which is also beginning to translate into applications. Approached holistically, these liquids therefore enable new universal manufacturing techniques that provide solutions to the existing problems of nanomanufacturing, and beyond that will open completely new horizons and possibilities for controlling the growth and assembly of nanostructures.

Examples that illustrate the power of ILs and DES in the improved manufacturing of nanomaterials are explored, such as the synthesis of light phosphors with exceptional quantum yields, record-figure-of merit thermoelectrics, and efficient photocatalysts.

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Electrochemical methods for the development and investigation of novel materials

Arunas Ramanavicius
Vilnius University

Conducting polymers are versatile materials applied in various technological fields [1-5].

During this presentation electrochemical [1], chemical [3] and biochemical [4] synthesis of conducting polymers (CPs). CPs-based structures in the design of various types of electrochemical biosensors will be outlined.

The applicability of CPs development of glucose biosensors based on glucose oxidase (GOx) will be discussed. Enzymatic reaction catalysed by GOx can be applied for the initiation of polymerization of some conducting polymers. We have shown that this method is suitable for the synthesis of polypyrrole, polyaniline [4], polytiophene [5] and some other conducting polymer based layers and nanoparticles. We also have demonstrated that formed nanostructures and nanoparticles shows good biocompatibility with living cells and when they were injected in mice. We have demonstrated that during such kind of synthesis of nanoparticles and/or nanostructured layers the enzymes becomes entrapped within CP-layer. Applicability of CPs in the design of molecularly imprinted polymer based electrochemical sensors [5] will be discussed.

CPs-based nanoparticles and nanostructured layers are suitable for the design of bioelectrochemical devices.

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Catalyst-free metal oxide nanowire growth and application

Simas Rackauskas

Kaunas University of Technology

Catalyst-free methods are attractive for facile fabrication of pure nanowires without the need for catalyst preparation. Nonetheless, how nanowire growth is guided without a catalyst is still widely disputed. The aim of this work is to explain nanowire growth based on classic crystal growth mechanisms.

Nanowire growth dynamics were investigating with in-situ transmission electron microscope, using CuO NWs as a model material.

Metal oxide nanowires show good results for the application in UV sensing and antireflecting coatings.

Here, we show that the classic crystal growth mechanisms can implemented for explanation the nanowire growth during metal oxidation without the need of catalysts. Such unsophisticated nanowire synthesis opens wide prospects of application in sensing, antireflection coatings and other.

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Nanomaterial-based surfaces – promising alternatives to antimicrobial applications

Angela Ivask[1], Merilin Rosenberg[1], Vambola Kisand[2]
[1]University of Tartu, Institute of Molecular and Cell Biology
[2]University of Tartu, Institute of Physics

The highest level of microbial transmission occurs via frequently touched surfaces. Thus, fast elimination of contagious microbes from surfaces, e.g., by antimicrobially active surfaces is a key to combat the spread of infections. Scientific literature on antimicrobial surfaces has emerged since 1960s with copper was the first widely used active agent. Recently, a variety of formulations have been introduced to antimicrobial surface coatings in nanoparticulate form, to increase the active surface area and thus, antimicrobial efficacy.

In our group we have been developing nanomaterial-based light-activated surface coatings over several years (1-3). Such surface coatings are based on ZnO/Ag nanocomposites that compared with pure ZnO nanoparticles possess higher photocatalytic activity and thus, also elevated antimicrobial activity.

We have demonstrated the antibacterial efficacy of ZnO/Ag nanocomposite-based surfaces both, after direct spray-coating of the nanocomposites to surfaces as well as after their embedding to a polymer matrix. Depending on the test conditions, ≥99% reduction of bacterial counts on nanocomposite-containing surfaces has been achieved after 15-60 min. We have shown long-term stability and efficacy of the surfaces. Parallel cytotoxicity studies have indicated that the surfaces are safe for human use.

This work is expected to result in robust and effective photocatalytic surface coatings for external high-touch surfaces while also providing a framework for real-life relevant efficacy testing of antimicrobial surfaces in the future.

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Functional nanomaterials for biosensor and bone regeneration

Mikhael Bechelany

CNRS/European Institute of membrane

Engineered nanomaterials are resources designed at the molecular (nanometer) scale to take advantage of their small size and novel properties which are generally not seen in their conventional bulk counterparts. The two main reasons why nanomaterials can have different properties are: (i) the increase of relative surface area and (ii) the quantum confinement effects leading to novel optical, electrical and magnetic behaviors. In order to apply these nanomaterials in biofields and to increase the throughput of biobased nanostructured materials and devices for energy, environmental and health applications, an efficient immobilization of the biomolecules is needed by the control of the interfaces between the nanostructures and the immobilized biomaterials.

Here, we used different synthesis techniques [1-3] as the main tools for the creation of controlled nanostructured materials and interfaces in which the geometry can be tuned accurately and the dependence of the physical-chemical properties on the geometric parameters can be studied systematically in order to investigate their performances mainly in health applications.

We will show examples of how these methods can be used to create: (i) optical and electrochemical biosensors [4] and (ii) bionanocomposites materials for tissue engineering in which the performance varies with the nanostructures/interfaces [5].

This work opens perspectives for the use of these materials for industrial applications.

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Graphene for sensors and (quantum) electronics

Samuel Lara-Avila[1,2]

[1]Department of Microtechnology and Nanoscience, Chalmers University of Technology, 412 96 Gothenburg, Sweden

[2]National Physical Laboratory, Hampton Road, Teddington TW11 0LW, United Kingdom

Graphene and other two-dimensional materials are slowly reaching the market in a diversity of products including photodetectors, quantum standards, and composites.

Here I present an overview of graphene technologies based on a specific type of graphene, produced by heating silicon carbide at high temperatures, so-called epitaxial graphene on silicon carbide (or epigraphene).

The talk will focus on the production technologies for large-scale epigraphene and the use of this material for applications that we developed in the past 5 years in our group. These include using epigraphene as a superior realization of quantum standards, as well as sensors for chemical species, magnetic fields and terahertz waves. These developments have laid the foundations for large-scale production and electronic applications of graphene, and I will describe some of the already available commercial applications based on our results.

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Large Applicability of Polydopamine Coatings in Energy Production

Emerson Coy

NanoBioMedical Centre, Adam Mickiewicz University, ul Wszechnicy Piastowskiej 2, 61-614 Poznań, Poland

Until quite recently, polydopamine (PDA) was mainly applied as a surface initiator for several biomedical applications and as a "sticky" active component sensing platform. However, several previously overlooked properties of PDA have been coming to light as research on this material continues. In this talk, I will mainly focus on the role of PDA coatings in energy applications, such as its apparent universal role as a photosensitizer and its behaviour when in contact with a semiconductor [1]. I will introduce some of the main physicochemical aspects that make PDA an ideal coating for many photocatalytic applications, including results on a variety of semiconducting materials and nanostructures [2]. Finally, some of the recent findings and theories on the origin of this behaviour will be presented as well as some novel PDA architectures [3].

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Manipulation and characterization of individual nanostructures

Sergei Vlassov

Institute of Physics, University of Tartu, Estonia

When the structural unit of material is reduced to nanoscale dimensions, its specific properties and behavior start to depend on size and shape. It opens a route for fine-tuning the characteristics of materials and systems by precisely engineering the size and geometry of the structures. At the same time, it raises significant challenges both in theoretical description and in experimental investigation of nanoscale materials. Thus, reliable methods for characterization of individual nanostructures alongside with appropriate models capable of accounting for size and geometry effects are needed.

Our activities are related to the characterization and manipulation of individual nanostructures inside a scanning electron microscope (SEM) with the main emphasize on mechanical and tribological properties. The method is based on commercial and home-build nanomanipulation platforms equipped with a force sensor.

In my talk, I will give a brief overview of our nanomanipulation activities and will present chosen findings [1-4] related to unusual behavior of nanostructures in nanomechanical tests.

Characterization method based on a manipulation of individual nanostructures inside SEM provides a valuable real-time information on dynamic processes like crack formation and propagation. It also enables the assembly of nanoscale devices.

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Nanostructures for intracavity spatial filtering in microlasers

Kestutis Staliunas

Universitat Politecnica Catalunya (UPC) & Vilnius University (VU)

Microlasers (edge emitting lasers, microchip lasers) usually suffer from the poor spatial quality of emitted radiation, especially in high power regimes. Conventional techniques of intracavity spatial filtering are not applicable in such small-size devices. We propose the specially designed photonic microstructures (photonic crystals, micro-modulated thin films), to provide the intracavity spatial filtering, which due to their small dimensions (several micrometers of thickness) are especially useful in microlasers [1].

Especial challenge is the microfabrication of such structures – in inorganic material, of 3D modulation with a submicron modulation period. Up to now we used the direct laser writing [2], or atomic vapor deposition [3] to fabricate such filtering microstructures. However, the fabrication alternatives are highly desirable.

In the presentation I will show my online simulators of microchip lasers, and visually demonstrate how the simulated intracavity photonic microstructures improve the beam spatial quality. I will show the current experimental results as well. Presently the intracavity spatial filtering allow to improve the brightness of laser radiation by the factor of 3.

The search for the new contacts for fabrication alternatives and other technological issues, leading to new collaborations, is the main reason to participate in your conference.

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Multifunctional Chromogenic and Transparent Conducting Oxide Nanocoatings

José Montero[1], Seohan Kim[1,2], S. Anand[3], Pungkeun Song[4], Lars Österlund[1]
[1]Department of Materials Science and Engineering, Ångström Laboratory, Uppsala University, P.O. Box 35, SE-751 03 Uppsala, Sweden
[2]Materials Technology and Research, Pusan National University, Busan, 46241, Republic of Korea
[3]Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, Albanova University Center, SE-106 91 Stockholm, Sweden
[4]Department of Materials Science and Engineering, Pusan National University, Busan, 46241, Republic of Korea

Thin films with multiple functionalities are highly desirable. Examples include transparent coatings, where multiple physical properties must be met depending on application, e.g., conductivity (transparent-conductive oxides, TCO, for displays, low-emissivity coatings and electrodes), self-cleaning and heat management (solar energy and windows), and dynamic switching of transparency and colour modulation (chromogenic technologies for smart windows and displays). These coatings demand cooperatively acting multi-components pushing development of new materials and hybrid materials, as well as film deposition technologies. Here we show that functional inorganic coatings on transparent materials, fabricated by scalable and energy-efficient physical vapour deposition techniques, can be made using multi-layered functional transition metal oxide nanostructured thin films, nanocoatings. In the first part, we show two examples of advanced TCO nanocoatings: (1) Superficially oxidized, ultra-thin Ag-Pd-Cu films embedded between indium tin oxide layers in an oxide/metal/oxide configuration, yielding TCOs with superior transparency and maintained electrical conductivity [1]; and (2) nano-patterned indium tin oxide (ITO) embedded between thin amorphous ITO layers exhibiting selective suppressed thermal conductivity, with maintained electrical conductivity, excellent and adjustable transparency, yielding TCOs with high Seebeck coefficient and high Haacke's figure of merit, thus paving the way for thermoelectric functionalities of TCOs [2]. In the second part, we will focus on chromogenic materials, in particular on rare-earth oxyhydrides, which constitute a family of inorganic photochromic materials with promising applications in smart windows [3]. These oxyhydrides have been shown to be very stable in air and being able to retain hydrogen even when subjected to relatively high temperatures. Moreover, rare earth oxyhydrides exhibit very good photochromic optical contrast, dynamics and stability and could therefore be attractive alternative to conventional organic photochromic dyes. We discuss how such materials could be implemented as energy efficient window and display coatings.

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Organic-Composite Thermoelectrics: Balancing Performance, Sustainability and Ease of Synthesis

Simon Woodward, Yaoyang (Carl) Hu, Andrew T. Turley
University of Nottingham

For the last decade organic-composite materials have held out the promise of providing low cost, sustainable thermoelectric (TE) devices, for energy capture. Optimal materials are frequently doped multi-component blends. For example, while PEDOT-PSS can provide a power output of ~470 mW per m.K2 compositions containing additional PANI, graphene and carbon nanotubes can increase this to ~2700, above the performance of current commercial BiTe devices. Present levels of theory do not allow ab initio prediction of which blends of existing (or new) materials will provide excellent TE performance – leading to the need for new organic components/compositions to be discovered experimentally. Ideally, new organic TE materials should be prepared by sustainable chemistry using low energy routes. If not, non-deployable (due to monetary or environmental costs) easily result.

Synthetic organic/inorganic chemistry methods have been used aiming for efficient procedures. New materials have been synthesised and their TE properties measured.

Attaining sustainable organic TE materials is challenging: balancing synthetic needs against performance and sustainability, but attaining this will be vital for viable future TE technologies.

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Hydrogen storage: from nano materials to components

T. Klassen, M. Passing, L. Thi Tu, G. Gizer, C. Pistidda, J. Bellosta von Colbe, K. Taube, J. Jepsen, M. Dornheim

Helmholtz-Zentrum Hereon, Institute of Hydrogen Technology, Max-Planck-Str. 1, D-21502 Geesthacht, Germany Helmut Schmidt University, University of the Federal Armed Forces Hamburg, Holstenhofweg 85, D-22043 Hamburg, Germany

Hydrogen is the ideal clean energy carrier for our future sustainable energy economy as well as for zero-emission mobility. Recent research on materials for efficient reversible storage of hydrogen will be presented. Solid nanostructured hydrides offer a safe and energy efficient solution for stationary as well as mobile applications.

Highest energy efficiencies can be achieved, if working temperature and reaction enthalpy of the respective hydrogen releasing process can be tailored for the particular system integration, e.g. with a fuel cell. Tuning of reaction enthalpies can be facilitated using Reactive Hydride Composites (RHC), which release or store hydrogen by redox reactions between at least two hydrides. Different aspects from basic materials development to systematic scale-up and system design will be covered.

Evolut 4.0 Startup acceleration program

Romanas Zontovičius

Innovation and Entrepreneurship Development Department at Kaunas Science and Technology Park

Kaunas Science and Technology Park (Kaunas STP) is the largest innovation community in Lithuania. Over 110 companies are operating at the tech park. We cover the following industries: IT, Engineering, Health-tech, social innovation, future energy, and Green-tech. Here at Kaunas STP we assist start-ups and established companies on how to increase their transnational competitiveness, and consult them on business development, strategy, and other business-related topics. Park runs a 2-month startup pre-acceleration program called Evolut 4.0 which educates startup and helps to foster an innovation culture in the Kaunas region and Lithuania.

Speaker will provide insights for someone who is thinking of launching a startup acceleration program within their organization. For startups, it will be useful to hear the recommendations on when it is a good idea to participate in the acceleration program and when it's not, and how to pick the best one.

A Band Structure Engineering Concept Applied in Design of Novel Light Emitting Materials

Marco Kirm

Institute of Physics, University of Tartu, 1 W. Ostwald Street, 50411 Tartu, Estonia

In my talk I will discuss how publicly available electronic band structure calculation data can be applied in design of novel light emitting materials. In recent years, we have been studying ternary fluorides possessing ultrafast intrinsic emissions cross-luminescence and intraband luminescence [1, 2].

In order to investigate ultrafast emissions we have developed new setups for time-resolved luminescence spectroscopy, which were exploited at various beamline of synchrotron radiation centres MAX IV Lab (Lund, Sweden) and DESY Photon Science (Hamburg, Germany). The obtained results and challenges in such research will be discussed.

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Silicon micro and nanofabrication in the context of quantum optics

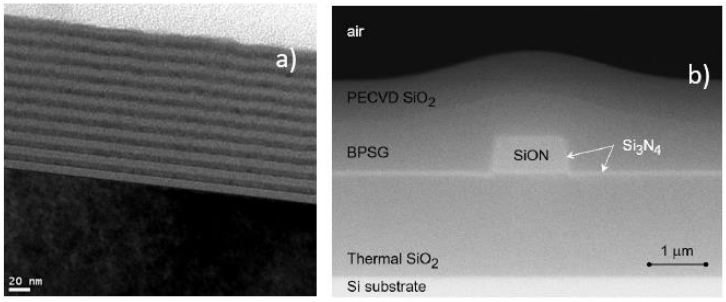
Georg Pucker, Gioele Piccoli, Martino Bernard, Mher Ghulinyan
Center for Sensors and Devices, Bruno Kessler Foundation, Italy

Keywords: silicon, nanocrystals, quantum random number generator, waveguides, simulation

The development of dedicated fabrication processes and engineering of materials plays also an important role in the context of quantum technologies. This is illustrated by presenting two examples of our research, which start with material, process optimization, and end with characterization of quantum devices. The first example is the use of silicon nanocrystal based light emitting diodes in combination with silicon photomultiplier detectors used to realize a quantum random number generators. The second is the development of a platform for a photonic quantum simulator based on nonlinear optical waveguides in SiON for generation of entangled photons and the integration of SiPM single photon detectors in the very same chip. The technology was applied for the integration of both P-I-N and SiPM detectors.

All key components used were fabricated with silicon microfabrication technology in Bruno Kessler Foundation. The Silicon nanocrystal based diodes were realized with a dedicated multilayer CVD deposition process and the layer thickness was optimized in the nanometer range to allow for injection of both electrons and holes, which allows for long time stability, low switch on voltage. The LEDs were carefully characterized and behaved as Poissonian light sources (single-photon emitter). On the other hand, a SiON waveguide was developed for operation from 780nm to 850nm. The waveguide was coupled efficiently to a P-I-N detector directly integrated into the same chip and the detection efficiency was estimated.

The Si-LEDS in combination with SiPM photodiodes were used to form a QRNG by observing the arrival time of photons continuously monitored by a FPGA. A post processing algorithm was used to correct imperfections in the electronic system and of the SiPM detectors. The QRNG passes all NIST tests for 2G random bits and achieves a maximum bitrate of 0.5 Mbps. On the other hand, we developed a SiON nonlinear waveguide with a Kerr coefficient of 1.6 +/- 0.2 dB/cm at 800nm and a Kerr-coefficient of 1.3 10^-19 m2/W, which is in between the values reported for SiO_2 and Si_3N_4. For the integrated P-I-N detectors a record quantum efficiency of 44% at 850nm is achieved, while with a similar integrated SPAD detector we can observe single photon detection.



High resolution TEM cross section of a annealed Si/ SiO_2 multilayer, b) SEM cross-section of a SiON waveguide

We show examples of the need for the optimization of materials and fabrication technologies to allow for realization of new quantum optical components.

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Peculiarities of dipolar ordering in mixed cation halide perovskites

J. Banys[1], S. Balciunas[1], M. Simenas[1], S. Svirskas[1], M. Kinka[1], V. Samulionis[1], R. Grigalaitis[1], A. Garbaras[2], A. Gagor[3], M.Maczka[3], A. Sieradzki[4]

[1]Faculty of Physics, Vilnius University, Sauletekio 3, LT-10257 Vilnius, Lithuania
[2]Mass Spectrometry Laboratory, Center for Physical Sciences and Technology, Sauletekio 3, LT-10257 Vilnius, Lithuania
[3]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, PL-50-950 Wroclaw, Poland [4]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, PL-50-370 Wroclaw, Poland.

The methylammonium (MA) lead halides $MAPbX_3$ (where X = I, Br, Cl) are popular perovskite materials among scientists and industry due to their perspectives in effective and cheap solar cells [1]. During the past decade, the power conversion efficiency of cells based on these hybrid compounds exceeded more than 20%. A high performance of these materials results from several physical properties such as large absorption coefficient, optimal bandgap, long carrier diffusion length, low exciton binding energy, exceptional defect tolerance. However, a successful application of hybrid perovskite solar cells is mainly prevented by their lead toxicity and poor both thermal and water stability. The most stable and efficient solar cells are obtained by using perovskites with mixed cations at the A-site. The most popular alternatives to MA are formamidinium and Cs^+ ions. A Dimethylammonium (DMA) cation has been introduced recently as an alternative A-site modification for these compounds.

Several investigations have shown that during certain synthesis procedures high quantities of DMA may be unintentionally introduced into $MAPbI_3$ and $CsPbI_3$. These modifications stabilize the preferable cubic phase of $MAPbI_3$ and leads to the enhanced performance at ambient condition. In the field of classical inorganic perovskites it is well known that mixing may significantly perturb structure of resulting compound. Thus, the long-range order can be suppressed and frustrated phases may appear.

The dielectric permittivity behavior of lead halides seem to be especially informative for the performance of the perovskite cells, as their relatively high value of the dielectric permittivity results in a pronounced defect tolerance and low exciton binding energy. However, a complete understanding of mixing effects on the dielectric permittivity dynamics and structural phase behavior is still absent. Here, we present a multitechnique experimental study of the mixed hybrid perovskite $MA_{1-x}DMA_xPbBr_3$.

Our results show that structural phase transitions are significantly suppressed even for a low substitution of the DMA cations. For higher DMA levels, the long-range dipolar order disappears and dipolar glass dielectric behavior dominates in the dielectric spectra.

Ultrafast material dynamics studies at the European XFEL

Andreas Scherz

European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany

The European X-ray Free-Electron Laser (FEL) is a high-repetition-rate X-ray user facility delivering soft and hard X-ray femtosecond pulses of unprecedented peak brilliance for studies in physics, chemistry, life sciences, and other disciplines.

Since fall 2017, six scientific instruments are in operation providing a diverse set of x-ray methodologies, and sample environments to address ultrafast processes in atoms, complex molecules, clusters or condensed matter. This talk will focus on out-of-equilibrium dynamics of complex materials and nanostructures in their fundamental space-time dimensions revealing the interplay of charge, spin, orbital and lattice couplings.

An overview of the employed X-ray techniques and capabilities in the soft and hard X-ray photon energy ranges will be given along with recent scientific examples of laser-driven phase transitions and magnetization dynamics of strong spin-lattice-coupled nanostructures. The presentation will conclude with a brief outlook to new capabilities of the XFEL and the instruments.

On-chip source of polarized single photons with orbital angular momentum

Shailesh Kumar[1], Mr Cuo Wu[1], Yinhui Kan[1], Danylo Komisar[1], Zhiming Wang[2], Sergey I. Bozhevolnyi[1], Fei Ding[1]

[1]Centre for Nano Optics, Mads Clausen Institute, University of Southern Denmark, Campusvej 55, DK-5230, Odense M
[2]Institute of Fundamental and Frontier Sciences, University of Electronic Science and Technology of China, Chengdu 610054, China

To obtain entanglement between orbital angular momentum (OAM) states and polarization states of single photons.

Color centers in nanodiamonds are sources of single photons at room temperature. We couple such single-photon emitters (SPEs) to surface plasmon polaritons (SPPs) supported on silver surfaces, by spin-coating nanodiamonds dissolved in deionized (DI) water. We further make dielectric Archimedean spiral gratings around the pre-characterized nanodiamonds containing SPEs.

A room-temperature on-chip integrated orbital angular momentum (OAM) source that emits well-collimated single photons carrying entangled polarization and OAM states is obtained. Two spatially separated entangled radiation channels with different polarization properties are generated. The OAM-encoded single photons are generated due to efficient outcoupling of diverging surface plasmon polaritons, excited with a deterministically positioned single-photon emitter, via Archimedean spiral gratings.

Our OAM single-photon source platform bridges the gap between conventional OAM manipulation and nonclassical light sources, enabling high-dimensional and large-scale photonic quantum systems for quantum information processing.

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Charge transport in topological insulator nanostructures

Gunta Kunakova
University of Latvia

In 3D Topological Insulators, due to the strong spin-orbit interaction, spin of the surface state electrons is locked perpendicularly to the momentum, and transport via the surface states is protected against backscattering from non-magnetic impurities. Exotic properties of the surface states in topological insulators are of great fundamental research interest and are attractive for applications in spintronics and quantum computing. Practically access and exploitation of the surface state charge transport is challenging to access due to the large contribution of the material bulk conductance, and one of the approaches is to use nanomaterials possessing large surface to volume ratio.

Magnetotransport measurements were conducted at a base temperature of 2K, in a Physical Property Measurement System, equipped with a 9T magnet.

Analysis of Hall effect measurements and Shubnikov-de Haas quantum oscillations confirms the presence of topological surface states. An additional band of high carrier density is identified and originates from an accumulation layer, formed at the nanoribbon/substrate interface. Charge transport exclusively via the surface states is achieved by gate-tuning the Fermi energy through the Dirac point. Alternatively, the formation of trivial accumulation layers interfering access the surface state transport can be mitigated in all-around encapsulated nanoribbons [2-4].

We conclude that topological insulator Bi_2Se_3 nanoribbons hold great promise for accessing new properties arising from the topologically protected surface states.

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Graphene-based sensors for environmental monitoring

Raivo Jaaniso
University of Tartu

Interest in low-cost sensors for detecting pollutants in indoor and outdoor environments has grown in recent years due to increased awareness of the harmful effects of these pollutants on health. As an extremely sensitive electrical transducer of molecular adsorption, graphene is an ideal platform for creating miniature sensors with unprecedented sensitivity.

To make such sensors selective to different gases, we developed the design principles of oxide-on-graphene structures using experimental and DFT methods. We functionalised single-layer graphene with a variety of ultrathin (down to 0.5 nm) oxide coatings (ZrO_2, V_2O_5, TiO_2, In_2O_3, Sc_2O_3, $CuMnO_3$) by pulsed laser deposition.

An overview of graphene-based gas sensors for environmental applications is given. Based on principles derived from empirical and theoretical data, we fabricated sensor arrays with different oxide-on-graphene structures. By applying machine learning to the array signals, different air polluting gases were simultaneously detected: NH_3 and H_2S, NO_2 and O_3.

Graphene is an excellent platform for creating miniature air quality sensors. Its full potential in environmental monitoring is further to be explored, together with related 2D materials and different functionalisation strategies.

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First-principles study of proton diffusion in $BaFeO_{3-\delta}$

Maximilian F. Hoedl[1], Andrew Chesnokov[2], Rotraut Merkle[1], Denis Gryaznov[2], Eugene Kotomin[1], Joachim Maier[1]

[1]Max Planck Institute for Solid State Research
[2]Institute of Solid State Physics, University of Latvia

Ceramic fuel and electrolyzer cells based on proton-conducting electrolytes usually employ a mixed electronic-proton-conducting cathode. While this ensures increased performance, it creates complex interactions between electrons and protons in the cathode material itself. Here, we explore the impact of these interactions on proton diffusion in cathode materials, specifically, in the $BaFeO_{3-\delta}$ perovskite system.

Density functional theory (DFT) calculations and nudged elastic band (NEB) method for the calculation of minimum energy paths and migration barriers of proton transfer.

Analysis of the electronic structure of $BaFeO_3$ shows that electron holes have a dominant O 2p character, so that a variation in hole concentration affects the properties of oxygen ions. This manifests in systematic variations of the oxygen vacancy formation energy and the material's propensity for water absorption as a function electron hole concentration [1]. Long-range diffusion of protons involves proton transfer between two neighboring oxygen ions that approach each other in a transient lattice vibration. The associated migration barrier is calculated as a function of oxygen vacancy (thus also electron hole) concentration. We observe systematic variations, which we describe by using various geometrical and electronic descriptors, and compare it to barriers in the $BaZrO_3$ electrolyte.

The proton migration barriers in $BaFeO_{3-\delta}$ show systematic variations with oxygen vacancy and thus electron hole concentration.

We are grateful for the computational resources by the HLRS DEFTD project (12939)

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First principles calculations of radiation defect properties in complex oxide crystals

Eugene Kotomin, Anatoli Popov, Vladimir Kuzovkov, Alexander Platonenko
Institute of Solid State Physics, University of Latvia

The radiation-resistant oxide insulators (Al_2O_3, $Y_3Al_5O_{12}$, $MgAl_2O_4$) are important materials for application in fusion reactors, e.g. as optical windows. For further prediction of the radiation stability of materials, it is necessary to determine main kinetic parameters - interstitial migration energy and diffusion pre-exponent.

The basic theory was presented in ref. [1,2]. It was showed that the correlation of diffusion parameters in strongly irradiated oxides satisfies the Meyer–Neldel rule (MNR) [2] observed earlier in glasses, liquids, and disordered materials.

We performed defect computer simulations combining the first principles calculation of the atomic, electronic, structure and optical properties of advanced defective oxides with the kinetics of defect recombination upon annealing. We performed large scale computer calculations of basic defects and analyzed available experimental kinetics of the F-type electronic and V-type hole center annealing for three different ionic solids: neutron/ion-irradiated Al_2O_3 (sapphire) [1-3], ion-irradiated $Y_3Al_5O_{12}$ (YAG) [4,5] and $MgAl_2O_4$ spinel [6], all three wide gap insulating materials but with different crystalline structures.

In sapphire upon an increase of radiation fluence, both the migration energy and pre-exponent are decreasing, irrespective of the type of irradiation. This is MNR with normal dose dependence. For YAG and spinel we have confirmed MNR, but the dose dependence is inverse. We discuss the cause of this phenomenon.

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SERS using Self-Assembled Nano Structures of Different Geometry. Special Case of Wires, Spheres and Triangles

A. Tamulevičienė[1], J. Jokšaitė[2], N. Khinevich[1], M. Juodėnas[1], T. Tamulevičius[1], S. Tamulevičius[1]

[1]Institute of Materials Science, Kaunas University of Technology, K. Barsausko 59, Kaunas LT-51423, Lithuania

[2]Physics department, Kaunas University of Technology, Studentų Str. 50, LT-51368, Kaunas, Lithuania

Silver and gold nanostructures are the main players in the field of optical sensors where surface enhanced Raman scattering effect is employed. By changing the plasmonic metal, nanoparticle shape, and size it is possible to tune the localized surface plasmon resonance position and therefore adjust the sensitivity for certain excitation laser wavelength. The current research shows how we can create SERS active layers for particular wavelength by adjusting the shape and size of nanoparticles.

Silver nanowires were synthesized using polyol synthesis as described in [1]. Spherical silver [2] and gold [3] nanoparticles as well as triangular gold nanoparticles [4] were synthesized using seed mediated growth methods. Optical properties in a range of 190-1100 nm were probed using Avantes spectrometer. Nanoparticle linear dimensions and its dispersion were analyzed using SEM Quanta 200 FEG (FEI). Random monolayer of nanoparticles was deposited on the surface of porous silicon from the liquid-liquid interface. Additionally, the patterns of nanoparticles were deposited using capillary assisted particle assembly on PDMS templates. SERS measurements of 2-naphthalene thiol were performed with 532 nm wavelength excitation (in Via spectrometer).

We have shown the efficient assembly of nanoparticles on the liquid-liquid interface and transfer of those layers onto solid support (porous silicon, PDMS).

We conclude that the analysis of SERS signal on the created structures using 2NT as analyte material was investigated and detection of concentrations down to 10-8M was demonstrated.

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The initiated chemical vapor deposition of tailored polymer thin films – Fundamentals to advanced functional applications

Stefan Schröder

Kiel University

Device miniaturization and the consequent need for new thin film materials on the nanoscale is a current trend in many application areas of polymers in research as well as industrial production lines.

The initiated chemical vapor deposition (iCVD) process enables the fabrication of tailord polymer thin films on the nanoscale and is able to keep up with these requirements. Solvent-free deposition on complex geometries and large-area substrates, high film quality and the ability to coat temperature-sensitive substrates are just some of the many advantages of iCVD.

The talk demonstrates the advantages of the iCVD process with regard to the development of new materials as well as the improvement of existing applications. This includes the fabrication of new gradient copolymer thin films with completely new chemical and physical properties [1] as well as the functionalization of gas sensors and soft organic conductors to improve the performance of these materials in high humidity [2]. Furthermore the deposition of electret thin films via iCVD is presented [3], which are applied in noval magnetic field sensors [4]. In-situ quadrupole mass spectrometry coupled to the iCVD process is applied to increase the overall process control for industrial applications and to obtain a powerful tool for the real-time investigation of the underlying reaction kinetics [5].

It turns out that the process provides new pathways for many application fields requiring precise film thickness control and high film quality.

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Nuclear Fusion Research in Lithuania – history and perspectives

Egidijus Urbonavičius

Lithuanian Energy Institute

Since 2006 Lithuanian Energy Institute (LEI) became involved in nuclear fusion research. In the beginning area of interests was very limited, but further LEI became more and more involved in such wide topic as fusion research.

Currently the topics covered by LEI are balometric analysis of experiments performed at JET facility. Neutron transport and radiation impact on the structures is investigated for JET and IFMIF-DONES facilities. Strength and structural analysis of components of W7-X facility was investigated, but the main activities currently investigated at LEI are safety and reliability assessment DEMO facility as well as analysis of influence of external events.

The presentation describes the history of Lithuanian Energy Institute involvement to fusion research and perspectives in this interesting field of science and technology.

Deep understanding of advanced optical and dielectric materials for fusion diagnostic applications

Anatoli I. Popov[1], Eugene A. Kotomin[1], Vladimir Kuzovkov[1], Aleksandr Lushchik[2], Aleksandr Platonenko[1], Eugene Shablonin[2], V. Seeman[2], Theo A. Scherer[3]

[1]Institute of Solid State Physics, University of Latvia, Kengaraga 8, Riga LV-1063, Latvia
[2]Institute of Physics, University of Tartu, W. Ostwald Str. 1, 50411 Tartu, Estonia
[3]Karlsruher Institut für Technologie (KIT), D-76344 Eggenstein-Leopoldshafen, Germany

The industrial progress of 21st century could greatly benefit from development and exploitation of fusion reactors producing environmentally clean friendly electrical energy. One of the key problems here is the need for new advanced materials able to operate under extreme conditions (high temperatures and intensive neutron/gamma radiation). Search for such optical and dielectric materials is an essential part of EUROfusion-Latvia association activities. In this talk, I will give a short overview of the most interesting results obtained in the framework two EUROfusion Enabling Research Project - "Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion applications (AETA)" (2019-2020) and "Investigation of defects and disorder in nonirradiated and irradiated Doped Diamond and Related Materials for fusion diagnostic applications (DDRM) – Theoretical and Experimental analysis " (2021-2023).

In a series of joint works by ISSP UL (Latvia), UT (Estonia) and KIT (Germany), radiation damage of some promising functional materials from the EUROfusion consortium priority list was studied under neutron, proton, heavy ion and gamma irradiation.

The optical, dielectric, vibrational and magnetic properties of numerous crystalline and ceramic materials were carefully studied.

Based on this study, we developed new theoretical methods able to evaluate and predict advanced materials functionality and radiation damage evolution under extreme conditions [1-4]

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Hyperbolic Phosphorescence Decay Kinetics: Empirical Formula and Theoretical Models

Sergii Ubizskii[1], Oleh Buryy[1], Volodymyr Degoda[2], Halyna Podust[2]

[1]Lviv Polytechnic National University

[2]Taras Shevchenko National University of Kyiv

The phosphorescence glow decay kinetics in solids was studied in a significant number of materials under the different types of excitation. It gets especial interest in last decades with growing interest to phosphors with so called persistent luminescence (PersL) and their application in many fields. It was found even in the middle of the 19th century, that the afterglow decay kinetics of many of irradiated phosphors is well described by the empirical Becquerel decay function I(t)=I_0 (1+ct)^(-d), where parameter c and d can be found from the approximation of experimental dependence. The integral glow intensity ∫_0^∞▒I(t)dt of the afterglow light corresponds to the net amount of stored energy (or dose of irradiation) in storage phosphor. But sometimes the power d becomes less than one and the Becquerel decay function becomes non-integrable which means formally that the light sum of phosphorescence becomes infinite that, of course, has no physical meaning.

It is exactly the case of YAP:Mn crystal being studied as storage phosphor for luminescence dosimetry by means of optically stimulated luminescence [1] as well as some other phosphors studied before [2].

Several approaches are known to explain the hyperbola-like kinetics with d < 1 [2-5], but till now there is no general understanding of this phenomenon.

The present work is devoted to analysis of theoretical models of processes occurring during the phosphorescence and to searching of their consistency with observed kinetics described empirically by non-integrable Becquerel function.

The work was partially supported by the NATO SPS Project G5647.

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Carbene-metal amides: an emerging class of highly efficient OLED emitters

Kaspars Traskovskis[1], Armands Ruduss[2], Sergey Belyakov[3], Kitija Alise Stucere[4], Aivars Vembris[4]

[1]Riga Technical University

[2]Riga Technical University, Faculty of Materials Science and Applied Chemistry

[3]Latvian Institute of Organic Synthesis

[4]Institute of Solid State Physics, University of Latvia

Linear two-coordinate metalloorganic complexes composed of coinage metals (Cu, Ag, Au), as well as electron accepting carbene and electron donating amide ligands have recently attracted great attention as highly promising low-cost emitters for organic light emitting diodes (OLEDs). These so called carbene-metal-amides (CMAs) possess ability of triplet excited state harvesting, which are enabled by efficient thermally activated delayed fluorescence (TADF) mechanism. Unique structural properties of this emitter class allow attainment of near-unity photoluminescence quantum yields and sub microsecond emission lifetimes, making compounds highly suitable for electroluminescence applications [1].

Here we explore structural modifications of CMAs, by introducing novel carbene chemical fragments. Namely, thiazoline and imidazole ligands were used. The corresponding CMAs were synthesized using Cu or Au central metal and carbazole-based amide electron donors.

CMAs based on thiazoline ligands exhibit dual emission from monomer and excimer states. When incorporated in OLEDs, this results in efficient single-emissive-layer white electroluminescence [2]. In the case of imidazole ligands yet unprecedented photophysical behaviour was observed, when auxiliary electron acceptors were introduced at the periphery of carbene moiety. Specifically, through-space charge transfer process was enabled, substantially decreasing the singlet-triplet energy gap thus lowering thermal activation barrier for TADF process [3].

Our results expand theoretical understanding and practical application directions for CMA emitters.

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ABSTRACTS

of the ORAL PRESENTATIONS

ELECTROCHEMISTRY OF NANOSTRUCTURED Bi_2SE_3 THIN FILMS IN AQUEOUS Li andNa ELECTROLYTE

Raimonds Meija[1], Vitalijs Lazarenko[1], Yelyzaveta Rublova[1], Jana Andzane[1], Vanda Voikiva[1], Arturs Viksna[2], Donats Erts [1]

[1] Institute of Chemical Physics, University of Latvia, [2] Faculty of Chemistry, University of Latvia

Keywords

Bi_2Se_3; anode; aqueous sodium ion batteries; $NaNO_3$

Actuality and aim

While lithium-ion batteries have dominated the field of electrical energy storage, at the moment they face issues, such as geographically localized mining sites as well as expensive and flammable electrolytes. A use of aqueous sodium ion electrolytes could significantly improve the price and safety of the batteries. The challenge for commercialization of this technology, is that most materials are not suitable as electrodes due to their insufficient electronic conductivity and electrochemical stability [1]. In this work we investigate Bi_2Se_3 thin films for their application as anode electrodes, using aqueous electrolyte.

Methods

Electrochemical measurements were performed, using a 3-electrode system in 1 M NaNO3 in a potential range (-1.0 V ÷ 1.3 V) (vs Ag/AgCl). To identify the chemical composition and morphology, energy dispersive X-ray spectroscopy, energy dispersive x-ray spectroscopy and scanning electron microscopy were performed.

Results

CV results show, that an unstable SEI layer forms in the first cycle at the potential 0.86 V. A long-term CV investigation consisting of 30 cycles with the scan rate of 1.0 mVs^{-1} showed a gradual degradation of the Bi_2Se_3 thin film, consistent with the EIS measurements [2].

Conclusions

This aqueous Bi_2Se_3 system showed up to two orders of magnitude increased diffusion coefficients compared to other anode materials in Na electrolyte-based systems as well as limited anode electrode degradation over 5 CVs and, and significant changes of the anode after 30 CVs [2].

Acknowledgements

This research was funded by the European Regional Development Fund (project no. 1.1.1.2/VIAA/3/19/522, “Nanostructured binder-free Bi2Se3/CNT anode electrodes for sodium-ion batteries”).

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MECHANISMS OF POLYMER SURFACE CHARGE FORMATION AND APPLICATION FOR ENERGY HARVESTING

Andris Šutka

Riga Technical University, Latvia

Keywords
polymer surface charge energy

Actuality and aim
The contact electrification (CE) of polymers has gained a vast attention in field of mechanical energy harvesting and related application for powering microdevices and portable electronics. Numerous concepts of triboelectric nanogenerator (TENG) devices have been demonstrated which exploits CE for harvesting mechanical energy. There are various sources of mechanical energy which can be harvested by TENG including biomechanical movement, water drops, ambient noise, wind, and water waves. The performance of TENG devices is governed by magnitude of surface charge, thus it is highly important to understand the mechanism of CE to develop materials which are tending to gain strong surface charge.

Methods
Three mechanisms are proposed for driving polymer CE: (i) electron transfer; (ii) ion transfer and (iii) material transfer. Electron transfer is believed to occur by overlapping electron clouds from two distinct polymers in contact. Ion transfer is considered between water adsorbate layers on two polymer surfaces due to different affinity. In other case the charged fragments of macromolecules (organo-ions) are being transferred. The organo-ions are formed due to heterolytic covalent bond break.

Results
Among proposed CE mechanisms, ion transfer mechanism seems to be reliable in case of water/polymer contact electrification, but not critical because the surface charge formation on polymers has been measured in complete absence of water. For this reason, discussion remains between the electron transfer and material transfer mechanisms. However, the series of experiments indicates that the electron transfer in polymer CE has minor role. Material (organo-ion) transfer is the main mechanism for polymer CE and thus the pathways for increasing the magnitude of surface charge can be defined based on polymer deformative properties.

HIGH RESOLUTION ANALYSIS OF NANOPARTICLE SPEED USING A MECHANICAL TIME-OF-FLIGHT FILTER

Pavel Solař , Kateřina Škorvánková , Jaroslav Kousal , Suren Ali-Ogly , Ondřej Kylián

Charles University, MFF, KMF, Czech Republic

Keywords
Time-of-flight filter, nanoparticle speed, gas aggregation source

Actuality and aim
The aim of this work is development of methods of analysis of nanoparticles (NPs) speed using a mechanical time-of-flight filter and the measurement of the actual NPs velocities under different deposition conditions. Understanding the trends and obtaining the proper speed values is very important for the understanding of e.g. the in-flight modification of the NPs where the speed determines the time the NPs spend in the modification zone or the NPs interaction with the substrate upon impact.

Methods
The NPs speed has been analyzed using a custom built mechanical time-of-flight filter and was coupled with SEM analysis of the deposits to determine the relation between size and speed.

Results
After successful development of the mechanical time-of-flight filter [1], the efforts have been concentrated on the analysis of NPs speeds at wide range of deposition conditions to understand how each deposition parameter influences the final speed [2]. These parameters included aggregation chamber pressure, deposition chamber pressure, magnetron current and orifice geometry. Also, the analysis has been improved to account for dependency of speed on NPs size.

Conclusions
The speed of NPs has been determined in dependence on process parameters and NPs size.

Acknowledgements
This work was supported by the grant GACR20-15405Y from the Grant Agency of the Czech Republic.

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HIGHLY REGULAR LASER-INDUCED PERIODIC SURFACE SILICON STRUCTURES MODIFIED BY MXene/TiO_2 HETEROSTRUCTURE FOR ENHANCED PHOTODEGRADATION

Igor Iatsunskyi [1], Lys Lys [2], Iaroslav Gnilitskyi [2], Oleksiy Gogotsi [3]

[1.] NanoBioMedical Centre, Adam Mickiewicz University, Poland, [2.] Adam Mickiewicz University, Poland, [3.] Materials Research Center, Ukraine

Keywords
silicon nanoripples; MXene; TiO_2; photodegradation;

Actuality and aim
Photocatalytic degradation is a new, eco-friendly, and performant technique for water purification. Si is photostable, inexpensive, nontoxic and photocatalytic active material which able to absorb visible and NIR light for the degradation of organic pollutants. To overcome the limitations of Si-based materials for environmental cleaning, photocatalytic heterojunction incorporating different functional species is the most widely used strategy. Newly 2D transition-metal carbides named MXenes pose excellent electrochemical behavior.

Methods
We produced here highly regular laser-induced periodic surface silicon structures (HR-LIPSS)- Ti_3C_2Tx-TiO_2 ternary system.

Results
Main structural, chemical and optical parameters of produced nanocomposites have been studied. The photo degradation tests have been performed as well.

Conclusions
We reported the photodegradation of nanoripples photocatalyst for R6G molecules. We investigates the synergistic effect of MXene decorated Si nanoripples produced by femtosecond for photocatalytic applications. It is demonstrated that the produced nanocomposites increase the photoactivity (photodegradation of R6G dye molecules) because of synergistic effect of MXene which increases the charge carrier separation and optical absorbance. The combination of these factors makes these nanostructures highly applicable in various photocatalytic applications. The produced photocatalyst has shown high stability and reproducibility.

Acknowledgements
The authors acknowledge the financial support from the project CanBioSe H2020MSCARISE2017 (Project number: 778157).

STRUCTURE AND OPTICAL PROPERTIES OF $ZnFe_2O_4$/ZnO CORE-SHELL NANOFIBERS, DEPOSITED BY COAXIAL ELECTROSPINNING

Roman Viter [1], Viktoriia Fedorenko [1], Karlis Grundsteins [1], Mikus Melderis [1], Agris Berzins [2], Viesturs Sints [3]

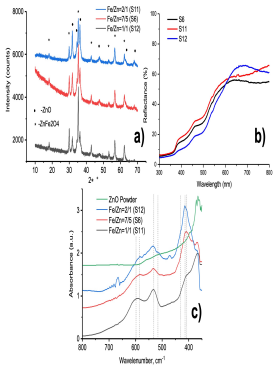
[1.] University of Latvia, Institute of Atomic Physics and Spectroscopy, Laboratory of Optical Biosensors and Functional Nanomaterials, [2.] University of Latvia, Faculty of Chemistry, [3.] University of Latvia, Institute of Physics

Keywords
metal oxides, core-shell nanofibers, coaxial electrospinning

Actuality and aim
Coaxial electrospinning is a novel technique for deposition of multicomponent nanofibers. Coaxial electrospinning is designed to form core and shell of different materials within structure of a nanofiber. Forming of composite material with low optical band core, active shell, stable interface and high surface to volume ratio could be important for advanced visible light photocatalysis.
In the proposed research we report on development of $ZnFe_2O_4$/ZnO core-shell nanofibers, deposited by coaxial electrospinning. Structure properties and optical properties have been investigated and analyzed as mass ratio of M[Fe]/M[Zn] in core shell precursors.

Methods
Iron and Zinc nitrates were added to 10 and 12 % solutions of PVP in DMF, respectively. The mass ratio of M[Fe]/M[Zn] in core shell precursors varied from 1:1 to 2:1. $ZnFe_2O_4$/ZnO core-shell nanofibers have been depos ited by coaxial electrospinning (20 kV, 15 cm, 200 rpm) and annealed at 600 °C for 2 hours.
Structure properties of the core-shell nanofibers have been investigated by XRD, SEM/EDX, FTIR, diffuse reflectance (300-800 nm) and photoluminescence (350-800 nm).

Results
SEM images showed nanofibers of 400 nm in diameter and 4 micrometers lengths. XRD analysis identified only Z nO and $ZnFe_2O_4$ phases. FTIR analysis showed the presence of Fe_2O_3 and Fe_3O_4 phases in the core material. Photoluminescence of the core shell nanostructures was low due to high rate of photoinduced charge separation. Diffuse reflectance showed absorption bands at 3.2, 2.5, 2.3 and 2.1 eV. Increase of M[Fe]/M[Zn] ratio resulted in increase of visible absorption and red shift of UV absorption band.



a) XRD of Fe/Zn, b) Diffuse reflectance, and c) FTIR of Fe/Zn core-shell nanofibers.

Conclusions
M[Fe]/M[Zn] ratio defines structure, electronic and optical properties of the core-shell nanofibers.

Acknowledgements
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THE ROLE OF MEDICAL LABORATORIES IN TRANSDISCIPLINARY RESEARCH PROJECTS ON BIOMATERIALS

Oksana Sulaieva, Oleksandr Dudin

CSD Health Care, Ukraine

Keywords
biomaterilas, medical laboratories, biomarkers, host-biomaterial interplay

Actuality and aim
Collaborative biomaterials research has become increasingly prominent nowadays. The range of novel biomaterials (BM) and tissue-engineered devices has been growing rapidly and need clinical validation for further implementation. This requires a proper assessment of biocompatibility, biodegradation, and possible functional effects of BM on cells, tissues and organisms of animals and humans [1] with the appropriate assessment of local host response and the use of various laboratory biomarkers [2]. Herein we discuss the capabilities of medical laboratories and their potential contribution to project performance.

Methods
An analytical review of current methods used for the assessment of host response to various biomaterials was conducted.

Results
A diverse spectrum of approaches is used for assessing host response to BM. In addition to evaluating morphological and immunological host response to BM, genomic, proteomic, and metabolomic studies are widely applied for discovering possible genotoxic effects of BM, their impact on gene expression, various signaling pathways [3]. Clinical chemistry and immunoassays biomarkers provide the understanding of systemic biomarkers reflecting visceral functions and metabolic circuits. This ensures the role of laboratory testing in transdisciplinary research projects. Besides involving medical laboratories in research projects provides the opportunity to compare 'gold standard" methods in terms of expected outcomes. Last but not the least, the robustness of laboratory testing is safeguarded by internal and external quality control.

Conclusions
A transdisciplinary approach is essential for fostering BM research, and the involvement of medical laboratories gives essential benefits.

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CONDUCTIVE PCL-MXENE ELECTROSPUN MEMBRANE: DEVELOPMENT AND BIOMEDICAL EVALUATION

Maksym Pogorielov [1], Kateryna Diedkova [1], Alexander Pogrebnjak [2], Oleksiy Gogotsi [3], Veronika Zahorodna [3], Viktoriia Korniienko [2]

[1.] University of Latvia, Latvia, [2.] Sumy State University, Ukraine, [3.] Materials Research Centre, Ukraine

Keywords

MXene, conductive materials, biomaterials, biocompatibility

Actuality and aim

Conductive biomaterials with appropriate structural and electrical properties are essencial for development of tissue engineering construction for nerve and cardiac tissues regeneration [1]. But effective combination of conductivity and biocompatibility is still not acieved [2].

Methods

Polycaprolactone (PCL) membrane was produced using electrospinning technique with following deposition of single-layed MXenes. SEM, TEM, HR-TEM, XPS, FTIR and conductivity were assessed for detailed structural and fuctional characterization of materials. Biocompatibility and antibacterial assays were used to evaluate biological properties.

Results

Electrospinning technique allows to produce highly porous membrane with fiber diameter ranges from 200 nm to 1.7 μm. Immobilization of MXene provide did not significantly changed the mambrane structural parameters but increase conductuvity depending on deposition numbers. FTIR and XPS measurements demonstrate formation of PCL-MXene composit materials that proved by HR-TEM. Deposition of MXene provide antibacterial properties for PCL membrane agaist S. Aureus and E. Coli during the 24 h of co-cultivation. Biocompatibility assay shown high biocompatibility and appropriate cell proliferation rate during 7 days of co-cultivation.

Conclusions

Our research demonstrate effectiveness of MXene deposition in PCL electrospun membrane for formation of conductive biomaterils that could be used in tissue engineering, flexible electronics in biomedicine and sensors.

Acknowledgements

Research was supported by H2020 MSCA-RISE project "Novel 1D photonic metal oxide nanostructures for early stage cancer detection" (778157) and project "Jauna fotoluminescences platforma Listeria mono citogēnu noteikšanai" 1.1.1.5/21/A/001

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LASER-MADE METAL NANOPARTICLES FOR SARS-COV-2 RELATED APPLICATIONS

Tomas Tamulevičius[1,2,3], Asta Tamulevičienė[1,2,3], Jaunius Mykolaitis[2], Mohamed A. Baba[1], Gazy Khatmi[2], Dainius Zienius[4], Raimundas Lelešius [4], Algirdas Šalomskas [4], Martynas Simanavičius[5], Laimis Silimavičius[5], Gintautas Gylys[5]

[1.] Institute of Materials Science, Kaunas University of Technology; [2.] Faculty of Mathematics and Natural Sciences, Kaunas University of Technology; [3.] UAB "Nanoversa", [4.] Faculty of Veterinary Medicine Lithuanian University of Health Sciences, [5.] UAB "Sanpharm"

Keywords

femtosecond laser ablation, gold, copper, nanoparticles, SARS-CoV-2, antivira

Actuality and aim

The need for fighting COVID-19 pandemics boosted related research activities and it turned out that various nanostructures could be used to inactivate the virus [1] or help to detect it [2]. The chemical synthesis of nanomaterials leaves some residuals of reactants or surfactants that can be fully avoided using photophysical synthesis. Pure metal targets immersed in a solvent and illuminated with the femtosecond laser turn into pristine nanoparticle colloids free from any contamination [3]. In this work, we aim to apply femtosecond laser ablated copper nanoparticles for developing antiviral surfaces and the gold nanoparticles are used for the detection of respiratory tract virus infections.

Methods

Yb:KGW femtosecond laser Pharos (Light conversion) was used to synthesize copper and gold nanoparticles in water from 99.9% purity targets. The beam was scanned by galvoscanner and focused with the f-Theta telecentric lens. The nanoparticle sizes were inspected with the field emission scanning electron microscope and the optical density of the colloids was evaluated with the UV-VIS spectrometer. The copper nanoparticles were spray deposited with an aerograph and their antiviral efficacy was tested against Bovine herpesvirus 1 (BHV-1) and Infectious Bronchitis Virus (IBV) Beaudette 18 strains. The prototype lateral flow immunoassay colorimetric detection tests were made using gold nanoparticles functionalized with anti-SCoV2-rN antibodies.

Results

Strongly absorbing copper and gold colloids of dark green and pink color were synthesized using laser ablation in liquid. The optical densities of ca. 10 at localized surface plasmon resonance peaks were reached after successive ablations of the 3x3 mm target area using 1-2 W power. The average nanoparticle size was 35 nm. Spray-deposited copper nanoparticles decreased the number of BHV-1 and IBV viruses by more than 96%. Antibody functionalized gold nanoparticles were successfully used to detect SARS-CoV-2 nucleoprotein down to 10 ng/ml

Conclusions

Copper and gold nanoparticle synthesis by using femtosecond laser ablation of metal targets appeared as a feasible method for developing antiviral surfaces and for applications in diagnostic lateral flow assays for detecting respiratory tract viruses.

Acknowledgements

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ANTIMICROBIAL ACTIVITY OF COMMERCIAL PHOTOCATALYTIC SANITISE WINDOW GLASS

Vambola Kisand, Meeri Visnapuu, Merilin Rosenberg, Dmytro Danilian, Sergei Vlassov, Mati Kook, Sven Lange, Rainer Pärna, Angela Ivask

University of Tartu, Estonia

Keywords
SaniTise; antimicrobial activity; TiO_2 coating; window glass;

Actuality and aim
At the end of 2020, Pilkington introduced SaniTise — a new pyrolytically TiO_2 coated glass. Pilkington states that this product "helps protecting against enveloped viruses and bacteria according to tests carried out by leading universities and independent laboratories"
In the current study, photocatalytic and antibacterial properties of TiO_2-based SaniTise glass by Pilkington were studied with an aim to benchmark this first commercial UVA-activated antimicrobial glass and to evaluate its efficacy in indoor-like conditions. For comparison, the antibacterial and photocatalytic activity of self-cleaning BIOCLEAN glass and photocatalytically inactive clear float PLANICLEAR control glass was analysed.

Methods
Photocatalytic activity measurements; XPS; AFM; SEM; Raman spectroscopy; Antibacterial tests by ISO 27447 and "dry droplet method";

Results
We confirmed the presence of anatase TiO_2 layer on the surface of SaniTise and observed significant UVA-induced photocatalytic degradation of a model organic dye.
In a liquid antibacterial assay corresponding to ISO 27447 format, 4 h exposure of bacteria to the SaniTise surface under UVA resulted in >2.8 log decrease in E. coli and >2.5 log decrease in S. aureus viable cell counts.
In experiments with the more application-relevant "dry droplet method", significantly higher antibacterial activity was observed up to the level where during 4 h at ≤ 50% RH complete inactivation of bacteria was observed.

Conclusions
Our results specify the need for more application-relevant test conditions and point to the fact that at low air humidity conditions, shorter exposure periods than recommended in the standard protocols should be targeted by photocatalytically active antibacterial surfaces.

SUPER-RESOLUTION MICROSCOPY AND THE SOFT DNA CURTAINS: HIGH-THROUGHPUT SM METHOD FOR PROTEIN-DNA INTERACTION STUDIES

Dr. Marijonas Tutkus [1], Aurimas Kopūstas [1], Mohammad Nour Alsamsam [1], Juste Paksaite [2], Meda Jurevičiūtė [2], Simonas Vytautas Ašmontas [2], Dr. Tautvydas Karvelis [2], Dr. Mindaugas Zaremba [2]

[1.] Institute of biotechnology, Life sciences Center , Vilnius Univ.; Department of molecular compounds Physics, Center for Physical Sciences and Technology, Lithuania, [2.] Institute of biotechnology, Life sciences Center , Vilnius Univ., Lithuania

Keywords

Super-resolution microscopy, Single-molecule DNA flow-stretch assays

Actuality and aim

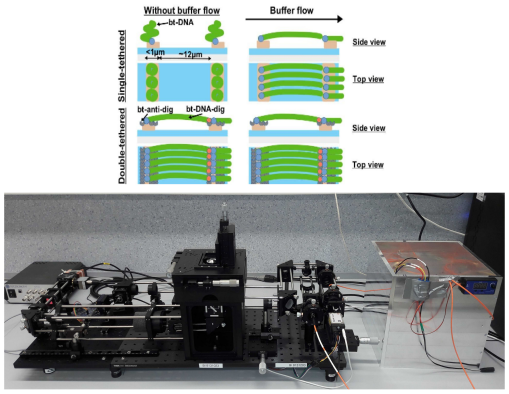
During the last 20 years, single-molecule fluorescence microscopy methods have evolved and widely spread. SM fluorescence methods enable monitoring various dynamic interactions. Next-generation in vitro SM biophysics approaches are characterized by a much greater complexity. One well-working method that belongs to the next-generation approaches is called DNA curtains.

Methods

Our Soft DNA Curtains platform for protein-DNA relies on stretching of long DNA molecules along the surface using the buffer flow. Biotin and dig labeled DNA molecules are immobilized on the nanoscale Streptavidin lines formed on the surface of functionalized glass coverslip. The second DNA end is tethered using bt-anti-dig antibodies. Our home-made fluorescence microscopy dedicated for super-resolution studies involves micro-mirror TIRF system, industrial-grade CMOS cameras, and Python-based microscope control and single-molecule localization microscopy data analysis packages.

Results

Our CRISPR-Cas protein-DNA interaction studies reveal differences in target-search mechanisms that these protein utilize. Development performed on the super-resolution microscopy and the related software allows us to perform cutting-edge microscopy.



Schematics of Soft DNA Curtains assay and our developed microscopy set-up

Conclusions

The novel Soft DNA Curtains platform can be applied to various DNA-interacting proteins. It is easy to use, efficient and reliable.

The microscopy set-up that we developed uses multiple efficient solutions and allows us to achieve < 30 nm resolution.

These developments can be easily applied in other similar studies performing laboratories.

Acknowledgements

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NITROGEN-DOPED MWCNTS WITH TEMPERATURE STABLE THERMOELECTRIC SENSITIVITY

Mikhail Katkov[1], Krisjanis Buks[1], Jana Andzane[2], Anatolijs Šarakovskis [3], Krišjānis Šmits[3], Donats Erts[2]

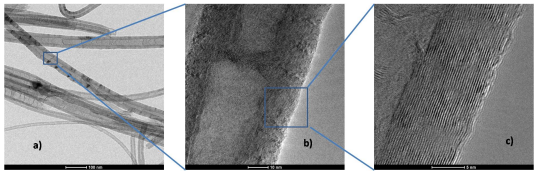
[1.] 3D Strong, LLC, [2.] Institute of Solid State Physics, University of Latvia, [3.] Institute of Chemical Physics, Faculty of Chemistry, University of Latvia

Keywords
carbon nanotubes synthesis, thermoelectrics, Seebeck coefficient, nitrogen

Actuality and aim
Carbon nanotubes (CNT) in networks create good electrically but not thermally conductive connections, making them favorable for thermoelectric applications [1]. Semiconductor electronics require the use of both p- and n-type semiconductors. While p-type CNT doping is easy, n-type CNT doping is more difficult in terms of itsstabi lity and overall device performance. An additional requirement for the modification method arises when the properties of CNTs must withstand high temperatures.

Methods
Nitrogen doping of multiwalled carbon nanotubes (MWCNT) allows changing nanotube properties through e lectron donating, which leads to n-type conductivity of the MWCNTs. For the thermal stability, the modification must be carried out during the growth of CNTs. Replacing carbon atoms by nitrogen is possible under Chemical Vapor Deposition (CVD) in terms of the temperature requirements [2].

Results
Thermoelectric sensitivity measurements show that MWCNTs doping by nintrogen under the CVD condition is efficient and leads to n-type behavior stable at elevated temperatures and persisting over a long period of time.



TEM images of N-MWCNT structures: a) low-magnification; b) higher-magnification ; c) close up

Conclusions
We describe a method for obtaining nitrogen-containing multi-walled carbon nanotubes under CVD conditions. We were able to synthesize n-type MWCNTs with stable Seebeck coefficients not reduced by thermal treatment in air.

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SYNERGY EFFECTS IN HYBRID EPOXY COMPOSITES WITH CARBON AND MAGNETIC NANOINCLUSIONS

Jan Macutkevic [1], Darya Meisak [1], Povilas Bertasius [1], Juras Banys [1], Polina Kuzhir [2]

[1.] Vilnius University, Lithuania, [2.] University of Eastern Finland, Finland

Keywords
carbon nanotubes, composites, nanoparticles, synergy effects

Actuality and aim
In this work epoxy resin composites filled with Ni@C nanoinclusion at various volume content were investigated in order to determine the electrical percolation and broadband dielectric/electric properties of these composites in a wide temperature range. Moreover, using the dielectric spectroscopy methods the properties of hybrid Ni@C/MWCNTs and MgO/MWCNTs epoxy resin composites materials were investigated in order to discover possible synergy between constituent components.

Methods
Dielectric properties of hybrid composites were investigated in wide frequency range from 20 Hz to 2 THz by means of the broadband spectroscopy. The sctructure of composites was investigated by the scanning electron mycroscopy.

Results
The dielectric/electric properties of the mono-filled Ni@C/epoxy composites with high volume Ni@C content (up to 30 vol.%) and hybrid Ni@C/MWCNTs/epoxy composites with fixed MWCNTs amount (just below percolation threshold in corresponding single-phase composites) and different Ni@C concentrations up to 1 vol.% were investigated in the broad frequency (20 Hz–40 GHz) and temperature (30 K–500 K) ranges. For mono-filled Ni@C/epoxy composites series, it was possible to roughly estimate the percolation threshold, which is in the range between 10 and 15 vol.%

Conclusions
Properties of epoxy resin composites with carbon natubes can be substantially improwed by addition of optimal amount of Ni@C or MgO nanoparticles. The dielectric analysis was also found to be effective tool for studing the distribution of nanoparticles in hybrid epoxy composites.

Acknowledgements
This presentation was supported by NATO project Certain.

X-RAY ABSORPTIONS STUDY OF CHROMOGENIC MATERIALS FOR SMART WINDOWS

Juris Purāns

Institute of Solid State Physics, University of Latvia, Latvia

Keywords
X-ray absorption spectroscopy, chromogenic metal oxides, smart windows

Actuality and aim
X-ray absorption spectroscopy (XAS) is an ideal non-destructive technique for characterising chromogenic materials, devices as well as for in-operando study chromogenic processes [1-3]. Synchrotron radiation XAS, comprised of both the high-resolution near-edge structure (XANES) and extended fine structure (EXAFS), is element sensitive to the local physical and electronic structure about both the metal (W, Ir, Mo, Ni, etc.) and oxygen target atoms in the chromogenic oxides.

Methods
Starting from our pioneering works in the 90s, we have applied XAS to the study of cathodic electrochromic oxides such systems as WO_3, WO_3-NiO, MoO_3, ReO_3-WO_3 [4] and to anodic oxides such as NiO_x, IrO_x, and recently ZnO-IrO_x, NiO-VO_x, NiO-IrO_x. In the study of thermochromic materials, XAS has been applied to $V(W)O_2$, $CuWO_4$-$ZnWO_4$, and recently, to the photochromic YH_3 and Y-O-H systems [3].
Here we examine chromogenic metal oxides of tungsten, molybdenum, iridium, nickel and mixed oxides and compare them to related crystalline species in order to set a foundation for the structure-property relationships in these oxides.

Results
In the amorphous electrochromic oxides (a-WO_3, a-MoO_3, a-ReO_3, a-IrO_x, a-Ta_2O_5, a-V_2O_5), the EXAFS analysis indicates the first coordination shell consists of oxygen atoms in a distorted octahedral geometry, with a second shell consisting of metals. No higher shells are observed beyond 3.5 Å for all samples, indicating the metal oxides are truly amorphous, consistent with X-ray diffraction results. While in the nanocrystalline anodic films (n-NiO, n-NiO-IrO_x), the EXAFS analysis indicates the structural peaks well visible up to 6 Å. The effect of size reduction is observed as a progressive decrease in peak amplitude upon increasing distance [2]. The oxidation state and local geometry of the metal centers in amorphous or nanocrystalline thin films of WO_3 (W^{6+}/W^{5+} oxidation state), IrO_x (Ir^{4+}/Ir^{3+}), Y-O-H (Y^{3+}/Y^{2+}) are determined using XANES spectroscopy.

Acknowledgements
Financial support was provided by ERDF Project no. 1.1.1.1/21/A/050.

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ALUMINUM NITRIDE – PERSISTENT LUMINESCENCE MATERIAL

Baiba Berzina, Rihards Ruska, Laima Trinklere, Janis Cipa

Indtitute of Solid State Physics, University of Latvia

Keywords
Aluminum nitride, luminescence spectra, luminescence mechanisms

Actuality and aim

Luminescent materials are with a great interest due to its many-side applications. Among them promising are the materials with a long lasting luminescence or the so-called persistent luminescence (PersL). Recently AlN:Mn was proposed as PersL material [1]. Our long term investigations of untreated and doped AlN allow revealing of luminescence mechanisms including the PersL mechanism, which is characteristic for this material.

Methods

In this research, the optical properties of materials were studied including measurements of photoluminescence (PL) spectra, its excitation (PLE) spectra and luminescence kinetics (LK) within a temperature range of 10 - 300 K, if necessary. It allows tracing down the optical processes, which follow the material irradiation with UV-visible light, resulting in emission of luminescent defects formed by the dopants-activators (ac) such as Mn or Eu ions or caused by the so-called oxygen-related (VAl - O) native defects.

Results

Analysis of the results obtained allows revealing of an intra-center luminescence (ICL) and recombination luminescence (RL) mechanisms schematically depicted on the figure below, demonstrating an energy level scheme of AlN containing different defects such as VAl-O, ac, oxygen and traps for electrons and holes. A detailed mechanism of the PersL is analyzed. This mechanism belongs to the RL basing on the thermo-stimulated (TS) processes when the electron-hole trap centers, which are filled during the sample irradiation, are involved.

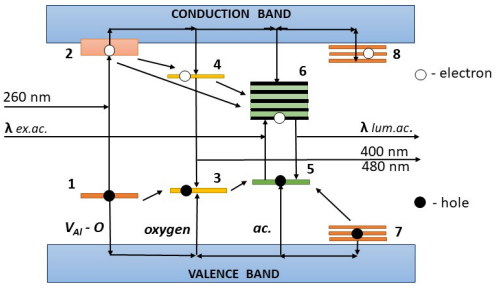


Fig. Energy level scheme of doped AlN illustrating luminescence processes and mechanisms.

Conclusions

A two-stage mechanism of PersL based on the tunneling and TS processes in AlN is proposed.

Acknowledgements

The financial support of Latvian Sciences Council Grant No. lzp-2019/1-0443 and CAMART^2 is greatly acknowledged.

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INFLUENCE TO HARDNESS OF ALTERNATING SEQUENCE OF ATOMIC LAYER DEPOSITED HARDER ALUMINA AND SOFTER TANTALA NANOLAMINATES

Helle-Mai Piirsoo, Taivo Jõgiaas, Peeter Ritslaid, Kaupo Kukli, Aile Tamm

University of Tartu, Insititute of Physics, Estonia

Keywords
nanoindentation; nanolaminates; atomic layer deposition

Actuality and aim
Ta_2O_5-Al_2O_3 nanolaminates are potentially applicable for high dielectric strength films [1], resistive switching material [2], and more. For most applications the mechanical properties of thin films have a significance on the reliability of the devices.
Double- and triple-layered amorphous Al_2O_3-Ta_2O_5 laminates with an overall thickness of ≈70 nm were atomic layer deposited while changing the sequence of the layers from surface to substrate to investigate the laminate structure's influence to hardness and Young's modulus.

Methods
The mechanical properties were studied by nanoindentation in continuous stiffness measurement mode.

Results
The laminates possessed hardness in a range of 8 – 11 GPa. Layered structure caused an uneven rise in hardness with depth dependent on the sequence and thickness of Al_2O_3 and Ta_2O_5 (Fig. 1). A tripleꟷlayered laminate and a quadruplelayered laminate possessed a steady change of hardness with similar values along the depth, although consisted of various amounts of oxides differing 3 – 4 GPa in hardness. The elastic modulus of the nanolaminates (145 – 155 GPa) did not depend on the structure [3].

Average hardness of triple-layered Al_2O_3-Ta_2O_5 laminates with topmost layer thicknesses presented.

Conclusions
The results indicate a possibility of nanoengineering a nanolaminate with a desired mechanical hardness by modifying the layer structure.

Acknowledgements
The study was partially funded by the European Regional Development Fund project "Emerging orders in quantum and nanomaterials" (Grant No. TK134), Estonian Research Agency (Grant Nos. PRG4 and PRG753) and ERDF project "Center of nanomaterials technologies and research" (NAMUR+, Project No. 2014-2020.4.01.16-0123).

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UPCONVERSION LUMINESCENCE IN ERBIUM DOPED TRANSPARENT OXYFLUORIDE GLASS CERAMICS

Anatolijs Sarakovskis, Guna Krieke

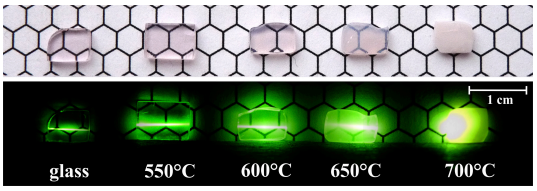
Institute of Solid State Physics, University of Latvia

Keywords
upconversion luminescence, transparent glass ceramics, oxyfluoride

Actuality and aim
From the application point of view, fluorides are the most perspective hosts for efficient upconversion luminescence (UCL) as they combine both low-phonon energy and chemical stability properties. Bulk transparent fluoride materials, however, generally are difficult to obtain, and often the UCL is studied in powders.
Oxide glasses, for example, silicates are perfectly suitable for applications where a transparent material is required, but they suffer from high phonon energy and the efficiency of the UCL in the RE doped glasses is very low.
Transparent rare-earth (RE) doped oxyfluoride glass ceramics composed of RE doped fluoride nanocrystals dispersed in glassy phase combines the advantages of both transparent glass and high efficiency fluoride phase. It possesses interesting and sometimes unique properties demanded by photoelectronics, telecommunications and solid state laser applications [1].

Methods
Differential thermal analysis, X-ray diffraction, Scanning electron microscopy, transmission electron microscopy, optical spectroscopy

Results
For the first time transparent erbium doped oxyfluoride glass ceramics containing hexagonal $NaYF_4$ nanocrystals has been prepared by melt-quenching and subsequent heat treatment of the precursor glass.



Glass and glass ceramics excited at 979 nm

Conclusions
The overall intensity of the upconversion luminescence of the glass ceramics sample is at least 200 times higher than that of the precursor glass. The observed enhancement of the efficiency is explained by the incorporation of Er^{3+} into low-phonon β-$NaYF_4$ crystalline phase. The relative intensity of the red upconversion luminescence band compared to the green band increases when the concentration of Er^{3+} is increased, which is explained by cross relaxation processes between activator ions.

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NANOSTRUCTURED THERMOELECTRIC MATERIALS SYNTHESIZED VIA SOLUTION CHEMICAL ROUTES

Bejan Hamawandi [1], Muhammet Toprak [1], Sedat Ballikaya [2]

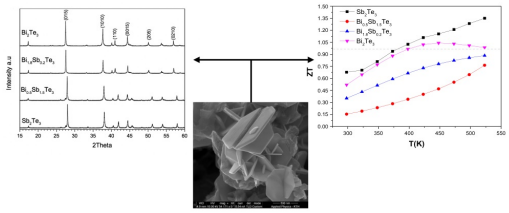
[1.] KTH Royal Institute of Technology, Sweden, [2.] Department of Physics, University of Istanbul, Istanbul 34135, Turkey

Keywords
colloidal synthesis,green chemistry, thermoelectric, nanoparticles

Actuality and aim
Thermoelectric (TE) materials are capable of interconverting between heat and electrical energy. Among the methodologies used to improve its TE properties, nanostructuring has been shown promising.

Methods
Solution chemical methods are bottom-up synthetic routes with significant advantages for synthesizing nanostructured TE materials with improved TE transport properties. The way In this work we compare the microstructure and resultant transport properties of nanostructured metal chalcogenides synthesized through different synthetic routes.

Results
Starting from available precursors and by means of energy efficient microwave-assisted heating, high purity nanostructured material is synthesised in very short reaction time -in a matter of few minutes, with controlled size, morphology, and surface chemistry. Three solution synthesis methods, in different solvents, namely hydrothermal, polyol and thermolysis were used to produce nanostructured TE powders. As-prepared materials are evaluated using XRD and SEM techniques.



Nanostructured $Bi_{2-x}Sb_xTe_3$ materials, structure,morphology and thermoelectric figure of merit.

Conclusions
TE transport properties are measured on pellets consolidated using spark plasma sintering process, through the evaluation of the electrical conductivity, Seebeck coefficient and the thermal conductivity. The TE transport properties are compared for same materials synthesized with different method to correlate the physiochemical properties of the synthesized materials with the synthetic route the material is made.

Acknowledgements
Swedish Energy Agency (43521-1), Swedish Research Agency Council (VR, 2018-03462), European Union's Horizon 2020 research and innovation program under the grant agreement No 863222.

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APPLICATION OF NANOSTRUCTURED MATERIALS FOR FLEXIBLE THERMOELECTRICS AND ENERGY-EFFICIENT BUILDINGS

Jana Andzane [1], Raitis Sondors [1], Davis Gavars [1], Margarita Baitimirova [1], Mikhail V. Katkov [2], Donats Erts [1]

[1.] Institute of Chemical Physics of the University of Latvia, [2.] 3D Strong Ltd

Keywords
Thermal insulation, metal oxide nanowires, thermal oxidation, thermoelectrics

Actuality and aim
EU buildings are responsible for ~40 % of energy consumption and 36 % of CO_2 emissions in the EU, which makes them the largest energy consumer in Europe. Thermal insulation of a building reduces its power consumption by up to 50 %. Additional embedding of thermoelectric modules in the thermal insulation panels would provide generation of electrical power at the temperature gradient ~ 10-30 °C, adding another 10 % to the reduction of the power consumption of building. The aim of this work is to develop environmentally friendly zinc and copper oxide based nanostructured thermoelectric materials, which may be built-in the thermal insulation panels for buildings.

Methods
Zinc/copper oxide nanowires are produced by the thermal oxidation of source zinc/copper [1]. Nanowire networks are fabricated by different methods as spray-coating, dielectrophoresis, mechanical transfer, followed by preservation of the resulting network by environmentally friendly or neutral binder. The characterization methods include electron microscopy, X-ray energy dispersive and photoelectron spectroscopy, as well as thermoelectrical measurements using custom equipment.

Results
Thermoelectric measurements of zinc/copper oxide nanowire networks showed significant values of Seebeck coefficient and electrical conductance and its dependence on the chemical composition of the nanowires, as well as on the quality of nanocontacts in the nanowire networks. Impact of different binders on the properties of metal oxide nanowire networks is studied.

Conclusions
Zinc/copper oxide nanowire networks showed significant potential for the development of energy-efficient solutions.

Acknowledgements
This work is funded by the ERDF project No. 1.1.1.1/20/A/144.

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NOVEL DOUBLE PEROVSKITES AND THEIR DERIVATIVES HOSTING RARE-EARTH IONS – A PRELUDE TO CHARGE TRANSFER PHENOMENON

Damian Wlodarczyk [1], Mikolaj Amilusik [2], Katarzyna M. Kosyl [3], Maciej J. Chrunik [4], Michal Strankowski [5], Volodymyr Tsiumra [3], Tomasz Giela [6], Marcin Zajac [6], Aneta Grochot [3], Anna Reszka [3], Andrzej Suchocki [3]

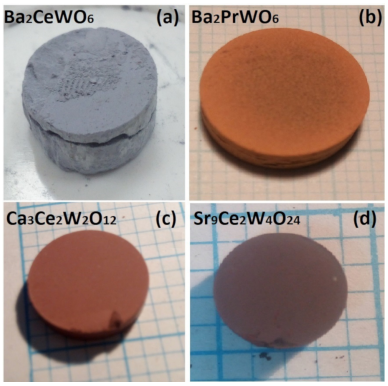
[1.] Institute of Physics PAS, Ave. Lotnikow 32/46, 02-668, Warsaw, [2.] Institute of High Pressure, Polish Academy of Sciences, Sokolowska 29/37, PL01142, Warsaw, Poland, [3.] Institute of Physics PAS, Ave. Lotnikow 32/46, PL02668, Warsaw, Poland, [4.] Military University of Technology, Gen. Sylwester Kaliski 2, PL00908, Warsaw, Poland, [5.] Gdansk University of Technology, G. Narutowicza 11/12, PL80233, Gdansk, Poland, [6.] SOLARIS NSRC, Jagiellonian University, Czerwone Maki 98, PL30392, Cracow, Poland

Keywords
double perovskites, ilmenites, charge transfer, photobleaching

Actuality and aim
Aim was to create new phosphors based on popular, efficient $BaWO_4$ scintillator doped with Ce or Pr in order to make a good energy down-converter with unique, controllable energy-transfer properties, but it actually turned out to be a weak phosphor with irreversible charge-transfer.

Methods
Powder XRD, SEM, XAS, XPS, EPR, Photoluminescence, Absorption.

Results
XRD showcased that Ba_2CeWO_6 and Ba_2PrWO_6 double perovskites share similar, small unit cells of I2/m SG and host unique charge transfer capabilities due to their specific Ce-W or Pr-W composition, respectively, confirmed by both XAS and XPS. This phenomenon is somehow connected to the presence of interstitial oxygen registered by EPR. Their large Sr^{2+} and Ca^{2+} cousins turned out to be tilted ilmenites (of I41/a and R-3c SG respectively) hosting many rare-earth shared sites with prominent defects that most likely stop electron free transfer within the matrix due to natural long-range energetical barriers. Photoluminescence shows complementary, weak but slowly decaying emission (withing several minutes) in first 2 of 4 aforementioned compounds while they are being exposed to 325-212 nm light or X-rays. SEM provides visual support for changing powders which were originally made in inert gas solid state reaction.



Visual depiction of newly created materials in form of pellets post Solid State Reaction.

Conclusions
Materials are considered to be relatively weak phosphors due to their unfortunate coloring and huge absorption followed by non-radiative heat dissipation. Yet still some of them show irreversible charge-transfer phenomena between luminescent-active ions withing the matrix turning them into effective NUV-Xray photobleachers that might find some use in future sensors development.

Acknowledgements
This work was founded by Polish National Science Centre Preludium 17 grant number 2019/33/N/ST5/02317.

STORY HOW USELESS THIN FILM THERMOELECTRIC GENERATOR BECOME ULTRA-FAST LASER POWER SENSOR

Martins Rutkis [1], Kaspars Pudžs [1], Jānis Busenbergs [1], Edgars Nitišs [2]

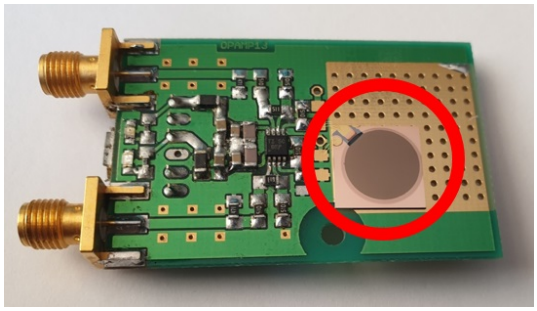
[1.] Institute of Solid State Physics, University of Latvia, [2.] Ecole Polytechnique Fédérale de Lausanne, Switzerland

Keywords
Thermoelectric materials, thin films, UV-VIS-IR laser pulse power sensor

Actuality and aim
The use of lasers in various fields of technology is inconceivable without precise control of their radiant energy. Current infrared (IR) sensors are not fast enough to record individual laser pulses. To overcome this shortcoming, technology was developed for a high-speed electromagnetic radiation sensor capable of characterizing a very short light pulse shape over a wide spectral range (UV-VIS-IR). The advance of the developed thermoelectric sensor is ensured by the use of innovative materials and technologies.
During my presentation, I will talk about the set of circumstances that allowed us to turn the concept of impractical thermoelectric generator created within the EC 7FP FET project into a patentable radiation sensor technology TESS.

Methods
Thin film deposition, COMSOL modeling, UV-VIS-NIR spectroscopy, testing as laser power sensor

Results
TESS:
• has broad spectral range - from excimers to CO_2 lasers;
• in IR region it is 1000 times faster than currently used;
• technology patented in EU, US, Canada and China;
• licensing and technology transfer agreement signed with Thorlabs GmbH.



TESS TRL7 prototype

Conclusions
TESS can be used when laser power is necessary to control on individual impulse level. For example, in laser surgical equipment, where its use will permit precise control of the applied radiation energy and thus allow more safe and efficient manipulations.

Acknowledgements
Development of TESS was supported by:
EC 7FP FET project: "Waste heat to electrical energy via sustainable organic thermoelectric devices" - H2ESOT
ERDF activity SAM 1.1.1.1 project Nr.1.1.1.1/16/A/046 "Application assessment of novel organic materials by prototyping of photonic devices"

ERDF activity SAM 1.2.1.2 project KC-PI-2017/40 "Thermoelectric radiation sensor" (TESS)

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PREPARATION AND CHARACTERIZATION OF ELECTRODES FOR NA-ION BATTERIES: $NA_2FEP_2O_7$ AND $NA_{0.67}MNO_2$

Gints Kucinskis [1], Beate Kruze [1], Inara Nesterova [1], Julija Hodakovska [1], Gunars Bajars [1], Donats Erts [2], Guntars Vaivars [1]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Institute of Chemical Physics, University of Latvia

Keywords
Batteries, electrochemistry, nanocomposites, Na-ion, cathodes

Actuality and aim
Na-ion batteries are a more sustainable alternative to the Li-ion battery systems that currently dominate the energy storage. Many of the materials and structures used in Li-ion batteries can be transferred to Na-ion chemistry. However, many questions regarding the optimization of active materials and formulation of electrodes and electrolyte are still unclear [1]. This work studies two cathode materials – $Na_2FeP_2O_7$ and $Na_{0.67}MnO_2$ – and optimizes their formulations.

Methods
Selected cathodes were synthesized, their structure and electrochemical properties characterized as a function of carbon content, binder used in the electrode and presence (or absence) of SEI-stabilizing electrolyte additive FEC.

Results
We find that $Na_2FeP_2O_7$ is stable for over 500 cycles at 1 C if 1 M $NaClO_4$ electrolyte in propylene carbonate (PC) with 5 wt.% fluoroethylene carbonate (FEC) additive is used as an electrolyte [2]. Stability of $Na_2FeP_2O_7$ in water has also been studied. Moreover, we also show that TBA alginate binder can improve the capacity of $Na_{0.67}MnO_2$ electrodes while unfortunately not mirroring the positive impact on cycle life that Na alginate binder has [3].

Conclusions
The results provide new insights into optimization of electrode preparation and selection of electrolyte in Na-ion battery cells.

Acknowledgements
Part of research was funded by Latvian Council of Science, agreement No lzp-2020/1-0391 and is acknowledged by IN, BK and GV. For selected experiments on $Na_2FeP_2O_7$, Horizon 2020 research and innovation programme under grant agreement number 964251 (FET-Open project TRANSLATE) is acknowledged. Project CAMART² has received funding from the Horizon 2020 Framework Programme H2020-WIDESPREAD-01-2016-2017-TeamingPhase2 under grant agreement No. 739508.

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WHAT SILICA-BASED THIN FILMS COULD DO FOR AUGMENTED REALITY DISPLAYS?

Ainars Ozols [1], Gatis Mozolevskis [2], Edvins Letko [2], Martins Rutkis [2], Roberts Zabels [3]

[1.] EuroLCDs, Latvia, [2.] Institute of Solid State Physics, University of Latvia, [3.] LightSpace Technologies, Latvia

Keywords
Augmented Reality, Silicon Oxynitride, Reactive sputtering, Thin films

Actuality and aim
Augmented reality solutions is still plagued by inconsistent image due to differences in accommodation and vergence distances, which brings along blurred image at close rendering distances, eye-strain and relatively swift onset of visual fatigue. To mitigate imposed limitations, volumetric-type displays in form of multi-focal display architecture have been proposed [1]. The main element is stack of very fast response time of LC diffusers, which switch between optically transparent and highly light-scattering state [2]. In the current form the optical-diffusers exhibit relatively high intensity reflections, originating from refractive index differences of display components, which lowers the overall optical efficiency of the display module as well as interacts with bright ambient lighting – lowering the image contrast. Such behavior limits use cases of AR devices based on given optical architecture.

Methods
Applicability of magnetron-sputtered silica-based films as dielectric layers serving purpose of mitigating refractive index jump within the structure of LC optical diffuser elements was investigated. The materials were chosen due to ability to steer their effective refractive index by varying sputtering conditions.

Results
Silica -based thin films refractive index, thickness, uniformity and dielectric properties and other properties have been measured and their impact on the properties of the final integrated element stack has been compared and found superior to traditionally used polyimide and SiO_x films.

Conclusions
With reactive magnetron sputtering the refractive index of silica-based compounds can be varied from 1.5 to 2.0 which allows to perform excellent index-matching between air, ITO and other display structures.

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NANOSTRUCTURED ANISOTROPIC MULTILAYER COATINGS FOR THE MANIPULATION OF LASER RADIATION

Lina Grineviciute, Lukas Ramalis, Rytis Buzelis, Tomas Tolenis

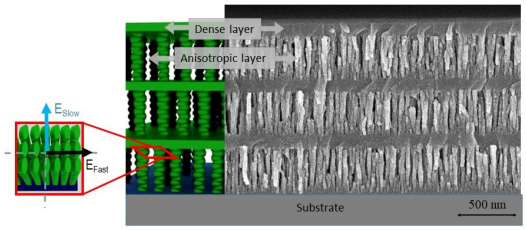
Center for physical sciences and technology, Lithuania

Keywords
Nanostructured films, optical coatings, physical vapor deposition

Actuality and aim
Optical elements for polarization control are one of the main parts in advanced laser systems. The state and intensity of polarized light is typically controlled by waveplates and polarizers. At high powers, both elements suffer low resistivity to laser radiation. Also, standard waveplates are fragile and difficult to use in small systems, while Brewster-type polarizers lead to light beam displacement in the optical path.

Methods
Physical vapor deposition; E-beam evaporation; Glancing angle deposition; Laser induced damage threshold measurements.

Results
The combination of birefringent nano-structured and isotropic layers allows to form zero-order wave-plates with desirable phase delay difference. Low optical losses and high transparency (T~99 %) are demonstrated while indicating potential to withstand high laser fluence of 40 J/cm^2 in nanosecond regime at 355 nm wavelength. Moreover, a novel multilayer approach to form all-silica polarizing coatings for normal incidence angle applications is proposed.



The schematic presentation combined with SEM image of the anisotropic coating cross section.

Conclusions
In this study, a novel multi-layer approach of high band-gap birefringent coatings was proposed and investigated. Zero-order thin film retarders and normal incidence polarizers based on all-silica nanostructures are fabricated by oblique angle deposition process. Low optical losses and the potential to withstand high laser fluence in nanosecond regime at 355 nm wavelength for both elements were demonstrated.

Acknowledgements
Research received funding from the Research Council of Lithuania (LMTLT), project UnCoatPower (agreement No S-MIP-20-61).

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PHOTOLITHOGRAPHY UTILIZING UP-CONVERSION LUMINESCENCE IN NANOPARTICLES MIXED WITH SU8 PHOTORESIST WITH/WITHOUT ORGANIC COMPOUNDS

Jurģis Grūbe, Kaspars Vītols, Viesturs Tenis Vīksna, Jānis Teterovskis, Jūlija Perveņecka, Ernests Tropiņš, Jeļena Butikova, Aivars Vembris

Institute of Solid State Physics, University of Latvia

Keywords
Up-conversion, luminescence, photolithography, nanoparticles

Actuality and aim
This work demonstrates a method which is essential to build up an experimental setup for the up-conversion (UC) luminescence photolithography system. Common photolithography method is when exposure is performed through the sample surface, but there is drawback - in thick samples, UV radiation is mostly absorbed in the upper layers of the sample, as the results deeper layers are unexposed. Such a problem can be solved when light emitting sources are placed into photoresist – like nanoparticles emitting UC luminescence (UCNP's). UC is a process in material, where absorbed light with low photon energy (IR), emits luminescence with higher photon energy (blue light or UV) [1].

Methods
UCNP's were synthesized by thermolysis method in two-day long process. UC luminescence was excited by 976 nm laser diode. The same laser diode was used for photolithography to record structures in system of UCNPs with SU8 photoresist with/without organic compounds.

Results
Intensive UV and blue up-conversion luminescence can be observed from synthesized nanoparticles with a hexagonal core ($NaYF_4$:Tm^{3+}, Yb^{3+})-shell ($NaYF_4$) structure (size ~35 nm) under IR excitation.

Conclusions
Several aspects have been considered to successfully develop and improve photolithography experimental setup to record structures in system of UCNPs with SU8 photoresist with/without organic compounds. The developed method is an alternative of a traditional i-line lithography. It is an innovative approach for recording of high-resolved three-dimensional structures.

Acknowledgements
This research is funded by the Latvian Council of Science, project "Up-conversion luminescence photolithography in organic compounds using nanoparticles/photoresist composition", project No. lzp-2019/1-0422.

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OPTICAL SPECTROSCOPY OF HIGH-QUALITY ZNO (0002) / CU (111) THIN FILMS GROWN BY ELECTRODEPOSITION

Ramūnas Nedzinskas [1], Artūras Suchodolskis [1], Laima Trinkler [2], Liuwen Chang [3], Mitch Chou [3]

[1.] Center for Physical Sciences and Technology, Vilnius, Lithuania, [2.] Institute of Solid-State Physics, University of Latvia, Riga, Latvia, [3.] Center of Crystal Research, National Sun Yat-sen University, Kaohsiung, Taiwan

Keywords
Photoluminescence; absorption; excitonic transitions

Actuality and aim
Zinc oxide (ZnO) is an attractive semiconductor material for near-ultraviolet (UV) optoelectronic devices, owing to the wide energy band gap (3.37 eV) and high exciton binding energy (60 meV) at room temperature. However, the major challenge for ZnO-based device applications lies in achieving the high-quality and stable ZnO of p-type. According to the recent scientific findings [1], group IB elements including copper (Cu) are suggested as the most promising to realise the p-type conductivity of ZnO.

Methods
In this work, optical properties of wurtzite-ZnO thin films, electrodeposited on Cu (111) substrate, are investigated using room temperature optical absorption (realised by using integrated sphere) along with excitation- and temperature-dependent (3-300 K) photoluminescence (PL) spectroscopy methods [2].

Results
Optical absorption allowed to investigate the excitonic absorption along with the bandgap energy of ZnO at room temperature under Kubelka-Munk approximation. The PL features observed are attributed to different processes of carrier dynamics in the ZnO thin film structures studied. In particular, the sharp high-energy feature is due to near-band-edge optical emission from ZnO epitaxial layer, while low-energy PL bands are related to the presence of defect states within energy band gap of ZnO.

Conclusions
Optical methods used allowed investigating the important fundamental parameters of ZnO thin films - band gap energy, activation energy, exciton-to-defect suppression. The optical parameters obtained are important feedback to adjust technological growth conditions.

Acknowledgements
The financial support of m-era.net project “ZnMgO materials with tunable band gap for solar-blind UV sensors” (ZMOMUVS) is acknowledged.

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COMPUTATIONAL METHODS FOR GUIDING PEAK ASSIGNMENT IN X-RAY PHOTOELECTRON SPECTROSCOPY

Juhan Matthias Kahk

University of Tartu, Estonia

Keywords
Density Functional Theory, X-ray Photoelectron Spectroscopy, ΔSCF

Actuality and aim
In core level X-ray Photoelectron Spectroscopy (XPS), core electron binding energies are measured to obtain information about the chemical composition of the near-surface region of the sample. The interpretation of core level XPS spectra relies on the assignment of detected peaks to atoms in specific chemical environments. Difficulties in making these assignments can limit the amount of information that XPS measurements provide. In order to overcome peak assignment problems, computational methods for predicting core electron binding energies have been developed.

Methods
In the Δ-Self-Consistent-Field (ΔSCF) method, the core electron binding energy is calculated as the total energy difference between the ground state, and the final state with an explicit core hole.

Results
In this talk, recent developments in ΔSCF calculations of core electron binding energies will be discussed, based on my previous work in this field [1-4]. I will first review the requirements for obtaining accurate absolute core electron binding energies in free molecules from first principles [2,4]. Next, I will discuss the application of the ΔSCF method to periodic solids [3], and adsorbates on surfaces [1,2].

Conclusions
Finally, future directions in computational X-ray Photoelectron Spectroscopy, including the routine prediction of XPS satellites, will be discussed.

Acknowledgements
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 892943.

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IMPACT OF SPIN-ORBIT INTERACTION ON STRUCTURE OF MATERIALS

Andris Gulans [1], Claudia Draxl [2]

[1.] University of Latvia, Latvia, [2.] Humboldt-Universität zu Berlin, Germany

Keywords
Density functional theory, spin orbit

Actuality and aim

The spin-orbit coupling (SOC) impacts the electronic structure of materials leaving a footprint on their chemical bonds too. This effect is pronounced in compounds with heavy elements giving rise to a volume change of up to several percent. Therefore, it is important to be able to account for SOC with a sufficient level of precision in calculations employing density-functional theory.

Methods

We implement a precise tool within a framework of linearized augmented plane waves in an all-electron full potential code exciting [1] and use it for comparing scalar-relativistic calculations with those including SOC.

Results

We consider three cases [2]:
(i) 45 elemental solids where we find that SOC induces the largest variation of the volume in Au, Tl, I, Bi, Po and Hg with the relative change ranging from 1.0 % to 7.6 %.
(ii) Group VA and VIIA dimers for which a bond-length extension is obtained. This effect is more pronounced for halogens than for pnictogens.
(iii) Two-dimensional Mo and W chalcogenides as well as groups IIB and IVA iodides. We find that whenever SOC has a detectable influence on chemical bonds, it alters their character making these materials less ionic. The strongest effect is observed for PbI_2, where SOC results also in a reduction of the lattice constant by 0.02 Å and a distortion of bond angles.

K 0.00%	Ca 0.00%	Sc 0.00%	Ti 0.00%	V 0.00%	Cr N/A	Mn N/A	Fe N/A	Co N/A	Ni N/A	Cu -0.02%	Zn -0.05%	Ga -0.05%	Ge 0.00%	As 0.03%	Se 0.35%	Br 0.39%	Kr N/A
Rb -0.03%	Sr -0.05%	Y -0.01%	Zr 0.01%	Nb 0.01%	Mo 0.04%	Tc 0.05%	Ru 0.03%	Rh 0.06%	Pd 0.06%	Ag -0.17%	Cd -0.33%	In -0.19%	Sn -0.03%	Sb 0.19%	Te 0.70%	I 1.49%	Xe N/A
Cs -0.10%	Ba -0.07%	Lu -0.72%	Hf -0.29%	Ta -0.05%	W 0.09%	Re 0.10%	Os 0.01%	Ir -0.12%	Pt 0.10%	Au -1.08%	Hg -6.71%	Tl -1.67%	Pb 0.12%	Bi 2.64%	Po 6.12%	At	Rn N/A

Relative change of volume in elemental solids due to spin-orbit coupling.

Conclusions

We provide precise data on the influence of SOC on chemical bonding and offer a qualitative explanation of this phenomenon.

Acknowledgements

The work has received partial support from the European Union's Horizon 2020 research and innovation programme, grant agreements No. 676580 (Novel Materials Discovery Laboratory) and No. 951786 (NOMAD CoE). We acknowledge also support from the German Research Foundation via SFB951, project number 182087777.

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ALN CERAMICS FERROELECTRIC PROPERTIES AND PHASE TRANSITIONS DYNAMICS

Edita Palaimiene [1], Jan Macutkevic [1], Juras Banys [1], Artyom Plyushch [1], Ewa Talik [2], Antoni Kania [2]

[1.] Faculty of Physics, Vilnius university, Sauletekio av. 9, LT-10222, Vilnius, Lithuania, [2.] Institute of Physics, University of Silesia in Katowice, UL 75 Pulku Piechoty 1, PL-41-500, Chorzow, Poland

Keywords
Ferroelectrics; piezoelectric properties; spontaneous polarization.

Actuality and aim
Promising materials for piezoelectric and dielectric applications are niobate based perovskites [1]. The aim of the work is to study ferroelectric and electrical properties of $Ag_{1-x}Li_xNbO_3$ ceramics via broadband spectroscopy, piezoelectric and ferroelectric polarization measurements.

Methods
Dielectric and IR measurements were performed in wide frequency range of 20 Hz - 750 THz, and several experimental techniques and apparatuses were used. For piezoelectric and ferroelectric investigations of ceramics TF Analyzer 2000E with a TREK 609E-6 4 kV voltage amplifier was used.

Results
Nature of the room temperature phase of ALNx ($x \leq 0.04$) ceramics is ferrielectric while for $x \geq 0.05$ ferroelectric. The frequency dependence of dielectric permittivity is mainly caused by the relaxational mode close to the ferrielectric/ferroelectric phase transition temperature and domains dynamics at lower temperatures. The strain versus electric field hysteresis loops measured for ceramics with $x \geq 0.02$ are presented in Fig.1. Moreover, their piezoelectric properties were also investigated and the highest piezoelectric coefficient value was observed for ALN_6. For ALN_x ceramics when $x \geq 0.06$ 15 polar modes were distinguished in the IR spectra and 20 polar modes for ALN_x ceramics with $x<0.06$, however the number or modes is temperature independent in investigated temperatures range (103-500 K).

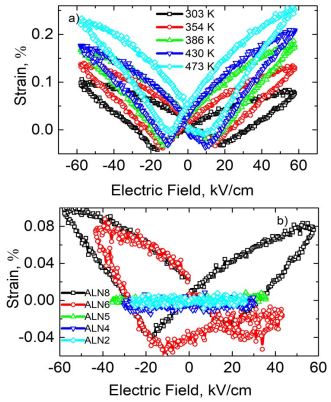


Fig.1.D(E) a) for ALN_8 at different temperatures; b) for ALN at different lithium concentrations.

Conclusions
In microwaves dielectric losses strongly increases with an increase in lithium concentration, indicating the impact of Li ions on the dielectric dispersion and phase transition dynamics in ALN. Extremely high value of d33=750 pC/N was observed at 465K for ALN_6, which makes the $Ag_{1-x}Li_xNbO_3$ solid solutions very attractive for high temperature piezoelectric applications.

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THE DECADE OF HYDROGEN: WHERE ARE WE HEADING TO?

Camila Pía Canales, Christiaan Richter, Rúnar Unnþórsson

Faculty of Industrial Engineering, Mechanical Engineering, and Computer Science, University of Iceland

Keywords
Hydrogen, electrolysis, seawater splitting, welfare analysis

Actuality and aim

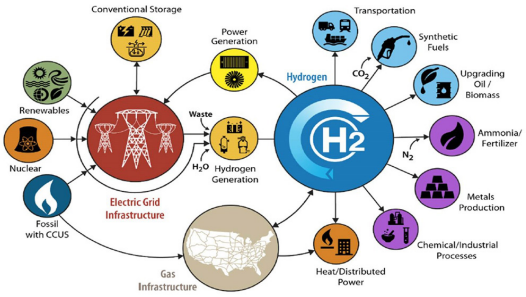
Global climate change is a scientifically well-recognized phenomenon and appears to be accelerated due to greenhouse gas (GHG) emissions such as carbon dioxide or equivalents (CO_2eq). Energy production remains a large factor in GHG emissions, contributing about 25 % of GHG emissions in 2010. To avoid more CO_2 emissions, methods such as electrolytic-produced hydrogen through water splitting, becomes a promising alternative as an environmental-friendly fuel. Yet, the scarcity of freshwater, makes some processes unsustainable, and the aim is to find sustainable ways to produce hydrogen from, for example, seawater, which can be used in many processes such as fuel cells. In this seminar, we will briefly discuss the underlying problems that come along when producing hydrogen using seawater and how we can optimize the existing methods. Then we will illustrate how theoretical and chemometrical studies through Bayesian Machine Learning can be implemented to combine diverse inputs like empirical data, welfare analysis and market-driven analyses to achieve insight into the socio-economic effects of introducing hydrogen as a clean energy carrier.

Methods

Chemometrical studies, in addition to laboratory studies, can be implemented to corroborate empirical data, as well as welfare analysis, to have a general idea of the socio-economic effects of introducing hydrogen as an alternative of clean energy.

Results

The available information in publications is still not clear.



Scheme of "hydrogen's big shot" (From PhysicsWorld and presented by Bryan Pivovar)

Conclusions

There are still some work ahead that must be addressed by understanding the underlying problems when using seawater as a resource for hydrogen production.

Acknowledgements

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APPLICATION OF BIOMIMETIC POLYDOPAMINE 2D-LIKE THIN FILMS FOR A SIGNIFICANT ENHANCEMENT OF ZNO AND TIO_2 PHOTOCATALYTIC PROPERTIES

Jakub Szewczyk [1], Marcin Ziółek [2], Igor Iatsunskyi [3], Katarzyna Siuzdak [4], Mateusz Kempiński [5], Fida Tanos [6], Mikhael Bechelany [7], Emerson Coy [3]

[1.] Adam Mickiewicz University, [2.] Faculty of Physics, Adam Mickiewicz University, Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland, [3.] NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614, Poznan, Poland, [4.] Centre of Laser and Plasma Engineering, The Szewalski Institute of Fluid-Flow Machinery, Fiszera 14 Str., 80-231 Gdansk, Poland, [5.] Faculty of Physics, Adam Mickiewicz University, ul. Uniwersytet Poznańskiego 2, 61-614 Poznań, Poland, [6.] Institut Européen des Membranes (IEM), UMR 5635, Université Montpellier, École Nationale Supérieure de Chimie de Montpellier (ENSCM), Centre National de la Recherche Scientifique (CNRS), Place Eugène Bataillon, 34095 Montpellier, France;, [7.] 2 Institut Europeen des Membranes, IEM, UMR 5635, Univ Montpellier, ENSCM, CNRS, 34730 Montpellier, France

Keywords
Air/water interface, semiconductors, degradation, functionalization

Actuality and aim

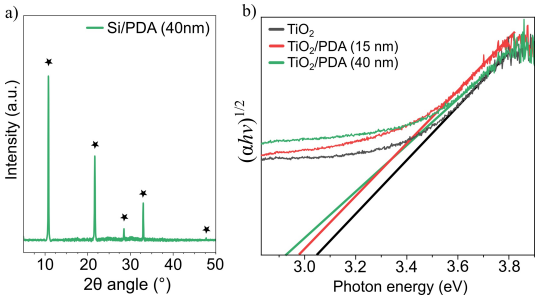
Despite notable scientific interest, polydopamine (PDA) free-standing films from the air/water interface have not yet been applied [1]. In turn, TiO_2 and ZnO have several disadvantages limiting their practical photocatalytic applications. In our experiment, we examine nanoscale-level combination of PDA with TiO_2 or ZnO towards photocatalytic performance enhancement.

Methods

The optimized films synthesis conditions were detailed in our recent work [2]. Obtained materials were examined by means of: X-Ray diffractometry, Raman Spetroscopy, X-ray photoelectron spectroscopy, Atomic force microscopy, transmission UV-Vis spectroscopy and Photoluminescence spectroscopy. The electrochemical methods used include: Light-sweep voltammetry, Cyclic Voltammetry, and Electrochemical impedance spectroscopy.

Results

Successful PDA deposition on the semiconductor interface was confirmed. Thereafter, we provide evidence of decreasing contribution of shallow defects in ZnO and TiO_2. Moreover, significant improvement of electrochemical properties and the charge carrier's recombination rate reduction was revealed. Finally, photocatalytic degradation of methylene blue show remarkable efficiency enhancement.



a) X-ray diffractogram of the PDA film on Si(100) substate
b) Tauc plot of the intrerface TiO_2/PDA

Conclusions

In summary, we significantly enhanced the TiO_2 and ZnO photocatalytic properties using versatile, easy-transferable and centimetre-scale biomimetic polydopamine free-standing films.

Acknowledgements

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MAGNETIC GOLD-COATED NANOPARTICLES FOR BIOANALYTICAL APPLICATION

Almira Ramanaviciene [1], Asta Kausaite-Minkstimiene [2], Anton Popov [2], Benediktas Brasiunas [2], Arunas Ramanavicius [2]

[1.] NanoTechnas - Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Lithuania, [2.] NanoTechnas - Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University

Keywords

Magnetic nanoparticles; preconcentration of biomolecules; signal enhancement

Actuality and aim

Nowadays, advances in nanoscience and nanotechnology open up new possibilities for the improvement of immunoanalytical system performance. Magnetic gold-coated nanoparticles (MNPs-Au) become more popular due to their properties characteristic to gold nanoparticles and the possibility to control their position with a magnet [1]. Thus, the possible ways of MNPs-Au modification with proteins and further application for immunosensing will be discussed.

Methods

The synthesis of MNPs-Au consisted of two parts - iron oxide MNP synthesis (using the co-precipitation method) and gold shell coating procedure. Antibodies on MNPs-Au were covalently immobilized via self-assembled monolayer formed on the outer gold layer.

Results

MNPs-Au modified with monoclonal antibodies were successfully applied for the separation of biomarkers from the relatively high volume sample and concentration into a low volume for further sensitive determination using biotin modified detection antibodies and streptavidin modified horseradish peroxidase [2]. Signal amplification strategy using MNPs-Au/antibody conjugates with surface plasmon resonance detection method was applied for the ultra-sensitive indirect detection of biomarkers [3].

Conclusions

The obtained results proposed the technical solutions for the development of the sandwich-type colorimetric magneto-immunoassay. The proposed SPR signal amplification strategy has advantageous properties and offers promising potential to significantly increase the sensitivity of immunosensors.

Acknowledgements

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SELF-ORGANIZED NANOSTRUCTURED METAL AND METAL OXIDE CONTAINING MULTILAYERS FOR OPTICAL SENSING

Juris Prikulis

Institute of Chemical Physics, University of Latvia

Keywords
porous anodic alumina, multilayers, electrochemistry, plasmonics

Actuality and aim
With a careful arrangement of nanostructures new hybrid architectures can be designed that combine multiple physical phenomena such as plasmonics, photoluminescence or interference effects, which can be useful for optical sensing. A viable way to produce such systems is to use self-organized structures e.g. porous anodic aluminum oxide (PAAO) as templates for deposition of other metal or metal oxide materials in different nanostructured multilayer architectures.

Methods
PAAO membranes were used as shadow-masks for metal nanoparticle deposition on glass surface [1]. PAAO with thickness below 300 nm was used to create hybrid metal-insulator-metal (MIM) type structures consisting of Al substrate, PAAO and porous Au film [2]. Alternative MIM structure was produced using capillary force assisted colloidal Au nanoparticle assembly on PAAO pore openings [3]. Using constant gradient variable thickness PAAO [4] and atomic layer deposition (ALD) technique aligned arrays variable length ZnO nanorods were produced [5].

Results
Au and Ag arrays created patterns of cross-polarized “hot spots” that were sensitive to refractive index changes and could be used for sensing without any spectral apparatus [6]. Nanoparticle arrays were successfully used as refractometric LSPR sensors and as SERS substrates [3]. Variable thickness PAAO allowed optimization of LSPR scattering by nanohole arrays [4] and use ZnO nanorods for sensing of vascular endothelial growth factor.

Conclusions
PAAO based nanostructured hybrid layers are very versatile and enable production of colorimetric and interferometric sensors, that employ different physical interactions with detectable materials. Change of PAAO geometry allows to tune and optimize the sensor performance.

Acknowledgements
LZP-2020/1-0200

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STRUCTURAL AND OPTICAL PROPERTIES OF OXIDE NANOPARTICLES AND NANOSTRUCTURES

Krisjanis Smits, Ivita Bite, Katrina Laganovska, Annamarija Trausa, Edgars Vanags, Liga Bikse, Virginija Vitola, Aleksejs Zolotarjovs, Donats Millers

Institute of Solid State Physics, University of Latvia

Keywords
nanocrystals, ceramics, luminescence, sensors

Actuality and aim
The presentation will summarize some previous research work completed over period of 20 years on oxide nanomaterials. Nanoparticles have emerged as key components in a wide range of applications in nanotechnology, nanoengineering, and nanoscience over the previous few decades. Nanoparticles are a good raw material for future applications, but the formation of defects must be properly studied.

Methods
The presented research will give an insight into our spectroscopy and electron microscopy studies of oxide nanomaterials, where lanthanide ions were used as luminescent probes to get information about processes and defects in these materials.

Results
The biggest part of presented results is obtained from the study of zirconia (as the host material) doped mainly with the Eu, Pr and Er lanthanide ions. However, results of other oxide materials (HfO_2, TiO_2, Al_2O_3, MgO, SiO_2, ZnO) will be provided.

Conclusions
The particular researches shows the importance of proper nanosize material studies and are related to synthesis of nanocrystals, preparation of transparent nanostructured ceramics, studies of oxide coatings on metals, sensor applications, materials for bioimaging etc.

Acknowledgements
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AB-INITIO MODELLING ELUCIDATES MATERIALS TRENDS FOR ELECTROCHEMISTRY APPLICATIONS

Denis Gryaznov [1], Maximilian Hoedl [2], Rotraut Merkle [2], Eugene Kotomin [1], Joachim Maier [2]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Max Planck Institute for Solid State Research, Germany

Keywords
solid oxide cells, cathodes, protons, vacancies, holes, DFT+U, PBE0

Actuality and aim
Protonic ceramic fuel/electrolysis cells are attractive due to higher ionic conductivities compared to oxide ion conductors at 300-600 °C. Optimized cathode materials with mixed protonic and electronic conductivity are crucial for their performance. Ab-initio modelling yields a deeper atomistic understanding of the key parameters determining proton uptake.

Methods
Density functional theory (DFT) calculations based on Hubbard (+U) approach and hybrid PBE0 exchange-correlation functional as implemented in VASP and CRYSTAL.

Results
DFT calculations were used to calculate oxygen vacancy and proton defect formation energies in nonstoichiometric $La_{(1-x)}Sr_{(x)}FeO_{(3-d)}$ and $Ba_{(1-x)}Sr_{(x)}FeO_{(3-d)}$ perovskites [1,2], from which defect concentrations can be derived. The trends in defect formation energy from DFT agree with experimental observations: more favorable hydration energy for lower La and higher Ba contents. Interestingly, the formal Fe oxidation state (varying between 3+ and 4+) also affects the hydration energy. We present a detailed analysis of volume and local geometry changes. The electronic density of states indicates that holes are shared between Fe and O, which explains the effect of hole concentration on the hydration energy.

Conclusions
DFT calculations reveal specific features in the electronic structure and allow us to understand the origin of experimentally observed trends. Based on this, the proton uptake can be optimized in a targeted way for application in protonic ceramic fuel/electrolysis cells.

Acknowledgements
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PLASMA TREATMENT APPLICATION FOR GREEN HYDROGEN PRODUCTION VIA HYDROLYSIS OF WASTE ALUMINUM IN ALKALINE WATER

Sarunas Varnagiris, Marius Urbonavicius, Darius Milcius

Lithuanian energy institute

Keywords
Hydrogen, Plasma, Aluminum, Sodium hydroxide, Byproduct, Aluminum hydroxide

Actuality and aim
Aluminum (Al) is an important strategic material in Europe with various application areas. Unfortunately, this invokes a huge amount of produced waste Al. The innovative improvements should be introduced to keep the waste management progress. In this case, Al could be utilized for energy generation through hydrogen evolution from water on-demand bypassing the hydrogen storage challenges.

Methods
Different types of Al waste were modified using a low-temperature plasma treatment. The comprehensive analysis was done by XRD, SEM, EDS, and XPS techniques. H_2 production via the reaction of Al waste and alkaline water was investigated. A solid reaction byproduct was investigated as well.

Results
Plasma treatment reduced surface organic contaminants and increased the creation of polar groups enhancing H_2 production rate. SEM showed some small cracks on the powder surface. Performed tests showed H_2 production starts after 1 min of Al powder immersion into slightly alkaline water while alkali solution needs to be increased for Al chips. The reaction byproduct can be converted into the valuable gamma-alumina with a high BET surface area (250 m^2/g).

Conclusions
Plasma increased hydrophilicity of Al powder surface and greatly improved H_2 production yield. The effect of plasma on Al chips did not appear to be as good as on powder, and more alkali was required to obtain a similar yield of H_2. The reaction byproduct could be a promising precursor for the production of ceramics or catalyst substrates.

Acknowledgements
The authors acknowledge financial support from the Baltic Research Programme project No. EEA-RESEARCH-92 “Aluminum in circle economy - from waste through hydrogen energy to alumina“ – AliCE-Why” under the EEA Grant of Iceland, Liechtenstein and Norway (No. EEZ/BPP/VIAA/2021/5).

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RAMAN VIBRATIONAL SPECTRUM MODELING OF WATER SPLITTING ON MULTIFACETED PEROVSKITE NANOPARTICLES

Veera Krasnenko

Institute of Physics, University of Tartu, Estonia

Keywords
water splitting, strontium titanate, computer modeling

Actuality and aim
Various photocatalysts are presently being studied to increase the photocatalytic efficiency of water splitting to produce hydrogen as a fuel and oxygen as a medical gas.
The several parameters could be varied in order to obtain desired photocatalytic properties. For example, a noticeable improvement of water splitting products was found experimentally on the anisotropic facets of strontium titanate (STO) nano/crystals. A recent first-principle study [1] of water splitting on a stepped (facet) STO surface revealed three different adsorption sites on such a surface, demonstrating very different catalytic activity. The identification of intermediate products of water splitting on such surfaces is an important task; which can be carried out experimentally and theoretically.

Methods
The density functional theory calculations were employed using local density approximation as implemented in CASTEP and CRYSTAL computer codes.

Results
To identify optimal sites for water splitting, we performed first principles calculations of the Raman vibrational spectrum of the bulk and stepped surface of a thin STO film with adsorbed water derivatives. According to our calculations, the Raman spectrum of a STO surface differs from the bulk spectrum, which agrees with the available experimental data. We identified characteristic frequencies of two types of surface OH radicals.

Conclusions
Using our approach we could identify the characteristic vibration frequencies for the STO of the stepped surface and the chemisorbed derivatives of water on the surface.

Acknowledgements
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CRYOGENIC TEMPERATURE NANOELECTROMECHANICAL SWITCH

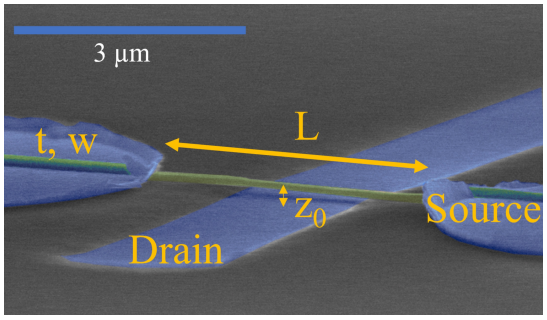
Liga Jasulaneca, Raimonds Meija, Edijs Kauranens, Raitis Sondors, Elza Dzene, Marks Prirodins, Donats Erts
University of Latvia, Institute of Chemical Physics

Keywords
Bi_2Se_3, nanoribbons, cryogenic, nanoelectromechanical switch

Actuality and aim
Cryogenic temperature operation of nanoelectromechanical (NEM) switches is interesting for various novel applications, such as in space installations, quantum computing and integration with superconductors. 3D topo logical insulator Bi_2Se_3 nanoribbons exhibit appreciable conductivity at temperatures as low as 2 K [1] and elas tic properties suitable for stress cycling, as demonstrated in situ [2], therefore they can be considered aspers pective candidates for cryogenic NEM switching.

Methods
NEM switches were fabricated on-chip using bottom-up grown Bi_2Se_3 nanoribbons as the active elements. Nanoribbons were integrated with metallic electrodes using scalable dielectrophoretic alignment and mechanical transfer methods. NEM switch operation was characterized in physical property measurement system.

Results
In this work, NEM switching at temperatures as low as 5 K was demonstrated [3]. Depending on the balance between adhesion and elastic restoring forces, volatile and non-volatile operation could be achieved. Switch-ON voltages of the as-fabricated devices were in the range of 5-27 V and were compared with those obtained with a combined analytical-numerical approach.



Schematics of a nanoelectromechanical switch, employing Bi_2Se_3 nanoribbon as the active element

Conclusions
The demonstration of NEM switching at cryogenic temperatures paves way for applications in sensors, memory and logic and can also serve as a means of exploring strain effects on topological surface states.

Acknowledgements
This research is funded by the Latvian Council of Science, project Topological insulator nanoelectromechanical current control devices for applications at cryogenic temperatures, project No. lzp-2019/1-0349. L. J. acknowledges the support of the University of Latvia patron “Mikrotīkls”.

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ENERGY AND SUSTAINABILITY: PROGRESS IN RENEWABLES AND ADVANCED "GREEN" NUCLEAR ENERGETICS

Andris Sternbergs

Institute of Solid State Physics, University of Latvia

Keywords
climate change, zero-carbon economy, renewables, nuclear energy sources

Actuality and aim
The Nobel Prize in Physics 2021 winners Syukura Manabi and Klauss Hasselmann helped science to better understand the Earth's climate and its effects on humans. Work of Giorgio Parisi on the other hand, allowed to better understand the interrelationships between various factors influencing the climate. He proved that even seemingly chaotic systems have hidden regularities that can be understood and explained.

Methods
With a focus on the transition to a zero-carbon economy, the energy crisis needs and energy independence issues to be addressed. As industry demands remain and even increase, the irregular nature of renewable energy has become a major problem. In this regard "green" nuclear energy as a long-term solution for baseload capacity is proposed as a complementary low-carbon renewable energy source. It is important that the development energy package in any country is based on the facts accumulated in the knowledge and experience

Results
There are two paths of obtaining nuclear energy:
- nuclear fission is the splitting of a heavy atom into two or more parts, releasing huge amounts of energy;
- nuclear fusion involves bombarding hydrogen atoms together to form helium and neutron.

Fusion is the same process that powers the sun and creates huge amounts of energy — several times greater than fission. It also doesn't produce highly radioactive fission products.

Conclusions
Nuclear power plants are the only source of carbon-free energy that can provide stable electricity day and night at any time of the year in almost any place on the planet.

Acknowledgements
H2020-WIDESPREAD-01-2016-2017-Teaming Phase2 under grant agreement No. 739508, project CAMART^2 are greatly acknowledged for financial support.

FUEL RETENTION IN ITER-LIKE-WALL JET PLASMA FACING COMPONENTS

Elina Pajuste [1], Gunta Ķizāne [1], Aigars Vītiņš [1], Anete Stīne Teimane [1], Līga Avotiņa [1], Andris Leščinskis [1], Mihails Haļitovs [1], Patrīcija Kalniņa [1], Rūdolfs Jānis Zabolockis [1], JET Contributors [2]

[1.] Institute of chemical physics, University of Latvia, [2.] EUROfusion Consortium, JET, Culham Science Centre

Keywords
Nuclear fusion, JET, ITER-Like-Wall, plasma facing materials, tritium

Actuality and aim
Nuclear fusion fuel, tritium T, accumulation in reactor breeding blanket and vacuum vessel materials is a key issue in terms of both tritium breeding self-sufficiency and safety of the fusion plant. In International Thermonuclear Experimental Reactor -ITER, limits of in-vessel tritium-inventory are an integral part of the ITER safety case and are fixed at 1 kg. ITER-Like-Wall project has been carried out at Joint European Torus (JET) to test plasma facing materials relevant to ITER [1].

Methods
Number of methods have been developed and applied in order to obtain comprehensive overview on tritium retention and behavior in plasma facing components. Results compared to deuterium data.

Results
Results revealed that the surface concentration of T of the plasma facing components of ITER-Like-wall were in a range from 1E10 to 1E14 atoms per cm^2. Its distribution pattern in the vacuum vessel is different from that for deuterium and is related to its accumulation as an energetic ion implantation in the materials in contrary to D main retention mechanisms - co-deposition. Energetic tritium ions are produced in D-D reaction, therefore, in D-T campaigns its contribution will be considerably smaller.

Conclusions
Results obtained within this study provides possibility to draw estimations on nuclear fusion fuel behavior in future fusion reactor materials.

Acknowledgements
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EXPERIMENTAL STUDIES OF THE 112SN(G,N)111SN AND 112SN(G,P)111M,GIN REACTIONS FOR P-NUCLEI PRODUCTION SIMULATION

Anastasiia Chekhovska [1], Nikolai Shul'ga [2], Anatoli Popov [1]

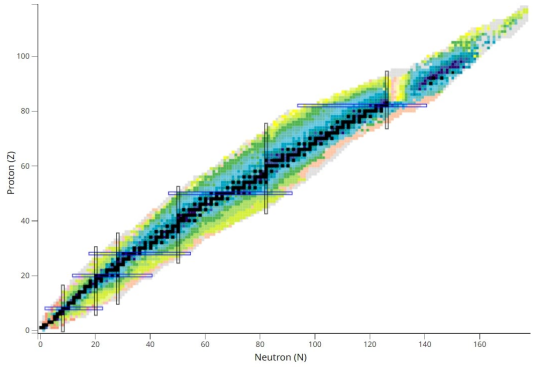
[1.] Institute of Solid State Physics, University of Latvia, [2.] National Scientific Center "Kharkiv Institute of Physics and Technology", Ukraine

Keywords
Photonuclear reactions; Radioactive decay; Bremsstrahlung; g-Ray emissions

Actuality and aim
The formation of radioactive isotopes is a major challenge for all materials in aggressive radiation environments, including diagnostic and design materials for fusion reactors (Eurofusion) and high-energy physics (CERN), as well as for space research.

Methods
The LINAC electron beam was converted to the bremsstrahlung which irradiated the targets. Gamma-activation technique was used for the experimental determination of the yields. The irradiated targets were delivered to the low-background region, where the spectra of g-decay quanta were measured using a high-resolution spectrometer based on HP(Ge)-detector.

Results
The yields of the photonuclear 112Sn(g,n)111Sn, 112Sn(g,p)111m,gIn, 114Sn(g,n)113Sn, 113In(g,n)112m,gIn reactions were determined. The experimental values of the yields agree with the theoretical predictions of the statistical theory of nuclear reactions in a diferent combination of models for the nuclear level density and the radiation strength function.
As an additional result, the new values of branching coefficients of the g-transitions following the decay of 111Sn nucleus are determined, which differ from the base (NuDat or LBNL) values by a weighted average coefficient of 1.38.



The lightest nuclei formed in interstellar space.

Conclusions
In this work using the activation technique we measured for the first time the experimental integral yields of the presented photonuclear reactions and compared them with the theoretical predictions. These experimental data can be used as input data in the g-scenario simulation computer codes for the astrophysical modeling of the stellar p-nuclei formation, and further improvement and parameterization of the statistical theory of nuclear reactions.

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3. DOI: 10.1103/physrev.87.366

DIETHYNYL FLUORENES AS PROMISING HEAVY-METAL FREE EMISSIVE MATERIALS

Anna Pidluzhna [1], Aivars Vembris [1], Raitis Gržibovskis [1], Oleksandr Bezvikonnyy [2], Dmytro Volyniuk [2], Juozas Grazulevicius [2]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Kaunas Technical University, Lithuania

Keywords
Diethynyl Fluorenes, luminescence, photoemission yield spectroscopy

Actuality and aim
Organic light-emitting diodes became very popular light sources during last decades because of numerous advantages. But there is a set of issues with OLEDs which needs to be solved and one of the problems is the application of heavy metals in metal-organic complexes as emissive materials. But most of heavy metals are toxic and some of them are already restricted in EU [1]. Therefore the synthesis of new efficient, heavy metal free electroactive emitters for OLEDs is one of the key tasks nowadays.
Fluorene derivatives are considered as promising emitters because of the good charge transport properties and high photoluminescence efficiency [2-3]. After n-buthyllithium and n-hexylbromide treatment of fluorine with bromine and $FeCl_3$ and after Sonogashira coupling [4-5] four different fluorene-based emissive substances 17b – 20b were obtained.

Methods
The film thickness was controled with use of Dektak 150 surface profiler. UV-vis-NIR absorption and photoluminescence spectra were measured with use of Ocean Optics HR4000 and fluorescence spectrometer FLS1000 respectively. All photoelectrical measurements were performed in high vacuum cryostat.

Results
These compounds demonstrate absorption maxima at 320-420 nm, emission maxima at 390-430 nm, 53-59 % of photoluminescence quantum yield for encapsulated samples, ionisation energy -5,9-6,2 eV, adiabatic gap -2.6-2,9 eV, electron affinity -2,9-3,3 eV.

Conclusions
According to obtained results the synthesised substances are attractive and promising for application in OLEDs.

Acknowledgements
The study was supported by VIAA project Nr: 1.1.1.2/VIAA/4/20/592

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SB_2S_3 SOLAR CELLS WITH COST-EFFECTIVE HOLE TRANSPORT MATERIALS FOR SEMI-TRANSPARENT APPLICATIONS

Sreekanth Mandati [1], Nimish Juneja [1], Atanas Katerski [1], Tatjana Dedova [1], Matas Steponaitis [2], Aiste Jegorove [2], Nicolae Spalatu [1], Aivars Vembris [3], Smagul Karazhanov [4], Vytautas Getautis [2], Malle Krunks [2], Ilona Oja Acik [1]

[1.] Tallinn University of Technology, Estonia, [2.] Kaunas University of Technology, Lithuania, [3.] Institute of Solid State Physics, University of Latvia, [4.] Institute for Energy Technology, Norway

Keywords
Solar Cells, HTM, Sb_2S_3, Semi-transparent, Fluorene, Enamine, Thiophene,

Actuality and aim
Due to its relatively wide bandgap, large absorption coefficient and excellent long-term stability, Sb2S3 has attracted increased research attention for thin film solar cells. However, their low efficiencies alongside the conventional expensive hole transport materials (HTM) like P3HT and Spiro-OMeTAD pose limitations on their commercial maturity. The present study unveils the use of cost-effective thiophene and fluorene-based HTMs towards semi-transparent Sb_2S_3 solar cells.

Methods
Solar cells of glass/FTO/TiO_2/Sb_2S_3/HTM/Au configuration are fabricated where TiO_2 and Sb_2S_3 are ultrasonic s pray deposited, respectively, whereas HTMs are spin coated.

Results
The cells with the new HTMs have demonstrated conversion efficiencies between 3.5-4.5 % on par with the cells with P3HT (4 %) as HTM. Further, the average visible transmittance (AVT) of solar cell stack with new HTMs without top electrode is > 30 % in 400-800 nm range qualifying them for semi-transparent applications. The cells with P3HT have yielded an AVT of ≈ 25 %. The band alignment reveals that new HTMs exhibit favourable band off-sets with Sb_2S_3 compared to P3HT.

Conclusions
Sb_2S_3 solar cells with considerable transparency and reasonable efficiencies are demonstrated using low-cost HTMs, which could have important implications going forward for semi-transparent applications.

Acknowledgements
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THERMAL, MECHANICAL AND ACOUSTIC PROPERTIES OF POLYDIMETHYLSILOXANE FILLED WITH HOLLOW GLASS MICROSPHERES

Tauno Tiirats [1], Sergei Vlassov [2], Sven Oras [3], Martin Timusk [4], Veronika Zadin [1], Ilya M. Sosnin [5], Rünno Lõhmus [2], Artis Linarts [6], Andreas Kyritsakis [7], Leonid M. Dorogin [5]

[1.] Institute of Technology, University of Tartu, Estonia, [2.] Institute of Physics, University of Tartu, Estonia, [3.] Tartu College, Tallinn University of Technology & Institute of Technology, University of Tartu, Estonia, [4.] Institute of Physics, University of Tartu & Research Laboratory of Functional Materials Technologies, Faculty of Materials Science and Applied Chemistry, Estonia, Riga Technical University, Latvia, [5.] Institute of Advanced Systems for Data Transmission, ITMO University, Russia, [6.] Institute of Technical Physics, Faculty of Materials Science and Applied Chemistry Riga Technical University, Latvia, [7.] Institute of Technology, University of Tartu

Keywords
PDMS; hollow glass microspheres; thermal conductivity; sound insulation

Actuality and aim

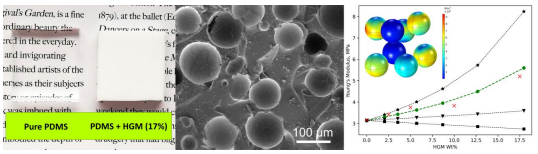
Polydimethylsiloxane (PDMS) is a widely used polymer due to its attractive properties [1, 2]. For example, it has a low thermal conductivity (~0.2 W/mK), which makes it already a good thermal insulator. Thus, most of the existing research tries to increase the thermal conductivity of PDMS. However, this work focuses on further decreasing the thermal conductivity.

Methods

Hollow glass microspheres (HGMs) were used as the heat insulating filler for the PDMS matrix. Sample range with HGM weight concentrations of 0 - 17 % were considered. The density, thermal conductivity, acoustic properties, wettability and mechanical properties of the samples were measured. Additionally, steady state Finite Element method (FEM) simulations were utilized to further analyze PDMS composite properties.

Results

The HGMs content had no considerable impact on wettability and sound insulation capacity decreased up to 3 dB for 5mm thick samples. With increase of HGM's concentration, the thermal conductivity reached 31% reduction and density reduced by 39% in comparison to pure PDMS, while Young's modulus increased approximately 60%.



Graphical abstract

Conclusions

By adding HGMs to the PDMS mixture a novel composite material with improved thermal insulating properties is created. The conductivity values obtained were still higher when compared to an alternative specially treated silica aerogel filler [3]. However, it benefits from simplicity of fabrication as it can be performed outside of laboratory conditions. Thus, the use of HGMs is a strong candidate for practical applications such as on-site preparation of a sealer with enhanced thermal insulation.

Acknowledgements

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ABSTRACTS

of the **POSTER PRESENTATIONS**

DETECTION OF X-RAY DOSES WITH COLOR-CHANGING HACKMANITES: MECHANISM AND APPLICATION

Sami Vuori [1], Pauline Colinet [2], Isabella Norrbo [1], Ralph Steininger [3], Timo Saarinen [4], Heikki Palonen [5], Petriina Paturi [5], Lucas C. V. Rodrigues [6], Jörg Göttlicher Göttlicher [3], Tangui Le Bahers [2], Mika Lastusaari [2]

[1.] University of Turku, Department of Chemistry, FI-20014 Turku, Finland, [2.] Univ Lyon, ENS de Lyon, CNRS, Université Lyon 1, Laboratoire de Chimie UMR 5182, Lyon, France, [3.] Karlsruhe Institute of Technology, DE-76131 Karlsruhe, Germany, [4.] University of Turku, Department of Geography and Geology, FI-20014 Turku, Finland, [5.] University of Turku, Wihuri Physical Laboratory, Department of Physics and Astronomy, FI-20014 Turku, Finland , [6.] Department of Fundamental Chemistry, Institute of Chemistry, University of São Paulo, São Paulo, SP, Brazil

Keywords
X-ray detection hackmanite inorganic photochromism tenebrescence

Actuality and aim

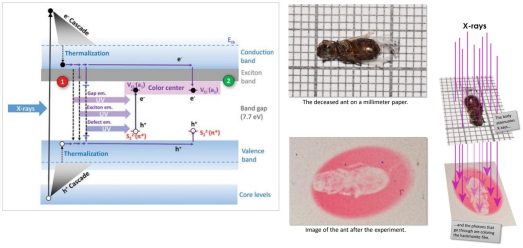
Hackmanite ($Na_8Si_6Al_6O_{24}(Cl,S)_2$) is a mineral that exhibits reversible coloration under UV irradiation. Thisco loration, also known as tenebrescence, stems from the formation of color centers that are created when an e lectron from a disulfur anion is raised to a chlorine vacancy with UV light. The structural rearrangement then creates a metastable color center which absorbs photons in the green part of the visible spectrum, rendering the color of the material pink [1]. This study focuses on same principle of coloration, which is now achieved with X-ray exposure. The studied materials were hackmanite samples where none or some of the Na was replaced with Li or Rb, or alternatively Cl was fully replaced with Br.

Methods

Synchrotron X-ray (coloration, XEOL). Reflectance spectroscopy. PXRD, electron bombardment and computational methods.

Results

The coloration is caused by a cascade of thermalized electron-hole pairs rather than direct valence electron detachment from sulfur. We also came up with an imaging technique, which exploits this tenebrescence feature.



The mechanism of X-ray induced coloration, and the tenebrescence imaging method.

Conclusions

The mechanism in X-ray-induced coloration in hackmanites was solved by combining different analytical methods.

Acknowledgements

Business Finland, SYSPROD project, AXELERA Pôle de Compétitivité, French agency ANR, FAPESP—São Paulo Research Foundation, Brazil, CNPEM, Centre Blaise Pascal's IT test platform at ENS de Lyon, Jenny and Antti Wihuri Foundation, Dr. Thomas Spangenberg.

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SYNTHESIS OF HIGHLY PHOTOCHROMIC HACKMANITE FROM NATURAL NEPHELINE

Cecilia Agamah, Mika Lastusaari

University of Turku, Finland

Keywords
Photochromic, hackmanites, natural nephelines

Actuality and aim

Photochromism, a phenomenon involving a reversible change of color upon exposure to a light or UV source has various applications such as UV dose determination, eye-protection glasses, energy-conserving coatings, optical switches, optical data storage devices, and privacy shield [1, 2]. The use of photochromic materials and systems are dependent on the rates of their optical transformations. For instance, very slow transformations are useful for optical data storage media, whereas fast transformations are required for optical switches[2]. Hackmanites, a promising and tunable optical multiplexing material has been a great area of interest over the last century because of its varied optical properties since it gives allowance to vary simple starting materials and temperatures to reach the desired optical properties [3]. We aim to tune hackmanites properties into various use by using simple but effective techniques with simple but cost effective starting materials.

Methods

We replaced Zeolite A (NaAlSiO4) (eq. (1)) with natural nepheline ($(Na,K)AlSiO_4$) and varied the metal chlorides, under simple synthesis method.

$6\ NaAlSiO_4 + NaCl + Na_2SO_4 \text{ --------> } Na_8Al_6Si_6O_{24}(Cl,S)_2$ .....(1)

Results

We have synthesized a highly photochromic hackmanite making the way to more ways to explore the uses of hackmanite and adding to it varied means of synthesis. These shows strong tenebrescence under 254 and 302 UV lamp and a weak tenebrescence under 365 nm UV lamp (Fig 1).

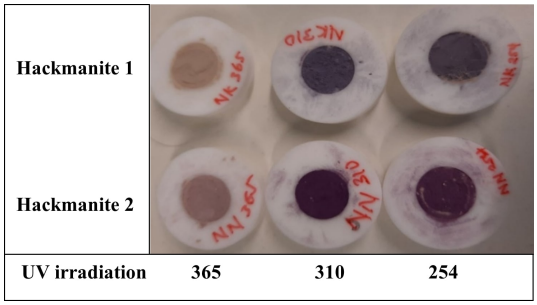


Fig 1. Coloration of hacmanites 1 and 2 under 365, 310 and 254 nm UV irradiation

Conclusions

We are currently investigating the properties of this material and are confident that just as the other hackmanites samples.

Acknowledgements

University of Turku

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NOVEL BROADBAND NEAR-INFRARED EMITTING LONG AFTERGLOW PHOSPHOR $MGGEO_3$: CR^{3+}

Guna Doke, Andris Antuzevics, Guna Krieke, Aija Kalnina, Anatolijs Sarakovskis

University of Latvia, Institute of Solid State Physics

Keywords
Persistent luminescence; TSL; EPR; Trap depth; Tunnelling; Cr^{3+}

Actuality and aim
For the last few years due to their potential application in some advanced fields such as anti-counterfeiting, night-vision surveillance, and especially bio-imaging, drug delivery and therapy [1-3], increasing attention has been devoted to near-infrared (NIR) persistent luminescence (PersL) phosphors. Therefore, we set our goal to develop and characterize a novel NIR emitting PersL phosphor.

Methods
Materials were synthesized by the solid-state reaction method and analyzed using optical and electron paramagnetic resonance spectroscopy experiments.

Results
A broadband NIR PersL signal was detected for more than 16 h after irradiation with UV. The traps present in material are closely overlapping with depth Ea ≥ 0.9 eV and the main detrapping mechanism in $MgGeO_3$: Cr^{3+} is athermal tunnelling directly to the Cr^{3+}.

Conclusions
The origin of the PersL is the $^4T_2(^4F) \rightarrow {}^4A_2(^4F)$ optical transition of Cr^{3+} ions substituting two non-equivalent Mg^{2+} positions in the host matrix.
The main trap centres responsible for PersL are intrinsic by nature and can be categorized into two types: oxygen vacancies serve as electron traps and oxygen ions serve as hole traps.
The $MgGeO_3$: Cr^{3+} material is a promising NIR persistent phosphor not only at room and higher temperatures but also at low-temperature conditions, which may be beneficial for applications in advanced fields such as anti-counterfeiting, night-vision surveillance, etc.

Acknowledgements
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PECULIARITIES OF THE LOCAL STRUCTURE IN A NEW HIGH-ENTROPY LOW-SYMMETRY (MNCONICUZN)WO_4 TUNGSTATE OXIDE

Georgijs Bakradze [1], Edmund Welter [2], Alexei Kuzmin [1]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Deutsches Elektronen-Synchrotron, Germany

Keywords
high-entropy oxide, tungstate, EXAFS, reverse Monte Carlo

Actuality and aim
The concept of high-entropy materials - first proven on metallic systems - now is actively being transferred to other classes of materials. Up to now only few attempts have been made to investigate HEM using X-ray absorption spectroscopy (XAS). XAS can be employed to probe fine structural effects in complex materials beyond the first coordination shell. For example, tungstates with a wolframite-type structure represent an interesting class of functional materials where new opportunities in XAS data analysis can be exploited. To the best of our knowledge, no attempts to investigate high-entropy tungstates have been made.

Methods
The phase purity and solid-solution nature were confirmed by X-ray powder diffraction and Raman spectros copy. XAS at the W L_3-edge and Mn, Co, Ni, Cu and Zn K-edges was used to probe the short-range-order in microcrystalline (MnCoNiCuZn)WO_4 powders. A structural model was obtained from a simultaneous analysis of the extended X-ray absorption fine structure (EXAFS) spectra at six metal absorption edges using the reverse Monte Carlo simulations.

Results
The composition-induced distortions of [WO_6] and [AO_6] octahedra in (MnCoNiCuZn)WO_4 at 10 K were evidenced from the shape of the W-O, and A-O radial distribution functions.

Conclusions
The obtained radial distribution functions for different atom pairs made it possible to investigate the local environment of metal ions and the effect of static disorder: on average, [AO_6] octahedra are less distorted, but more irregular than [WO_6] octahedra.

Acknowledgements
G.B. acknowledges the financial support provided by the State Education Development Agency for project No. 1.1.1.2/VIAA/3/19/444 (agreement No. 1.1.1.2/16/I/001) realized at the Institute of Solid State Physics, University of Latvia.

STRUCTURE AND STABILITY OF RADIATION DEFECTS IN $LiYF_4$

Jekabs Cirulis Andris Antuzevics, Andris Fedotovs, Uldis Rogulis

Institute of Solid State Physics, University of Latvia

Keywords
EPR, ENDOR, Radiation, Defects

Actuality and aim

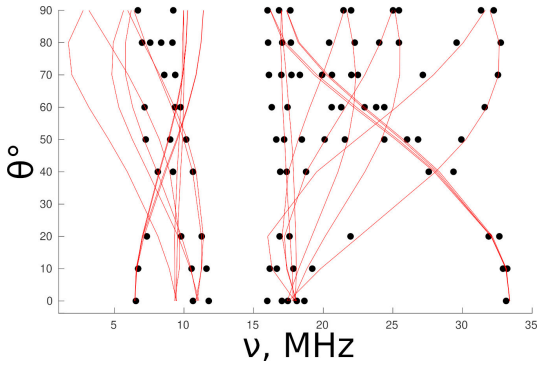
Scintillators are materials used for radiation detection and can therefore be exposed to intensive radiation [1]. As a result of exposure to ionizing radiation, the mechanical and optical properties of the material may be significantly altered.

Methods

Pre-synthesized LiYF4 single crystals were irradiated by X-rays. For irradiated samples, EPR and ENDOR spectra angular dependence was measured, rotating crystal around two mutually perpendicular axes. Samples were annealed at temperatures between 50°C and 400 °C to assess the stability of the defects by using EPR signal intensity as an indicator for the concentration of defects. Ab initio quantum chemistry program ORCA was used for local structure analysis of the defects.

Results

EPR and ENDOR spectra were used to determine spin-Hamiltonian parameters of the defects . A structural model of the defects can be proposed using obtained spin-Hamiltonian parameters values.



ENDOR spectra of oxygen X-ray defect in $LiYF_4$

Conclusions

It has been concluded that at least three EPR active defects are formed in irradiated X-ray $LiYF_4$ crystal, which anneal above 300 °C. One of the defects is an oxygen impurity and fluorine vacancy pair. Preliminary DFT calculations of the defect give a good approximation to experimental data.

Acknowledgements

Financial support provided by Scientific Research Project for Students and Young Researchers “Structure and stability of radiation defects in $LiYF_4$” realized at the Institute of Solid State Physics, University of Latvia is greatly acknowledged.

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DESIGN OF ANTIREFLECTIVE STRUCTURES FOR THE OPTICAL WAVELENGTH RANGE

Tomas Klinavičius [1], Tomas Tamulevičius [2]

[1.] Institute of Material Science, Kaunas University of Technology, Lithuania, [2.] Institute of Material Science, Kaunas University of Technology; Department of Physics, Kaunas University of Technology, Lithuania

Keywords
Subwavelength diffraction grating, metamaterial, antireflective, RCWA

Actuality and aim

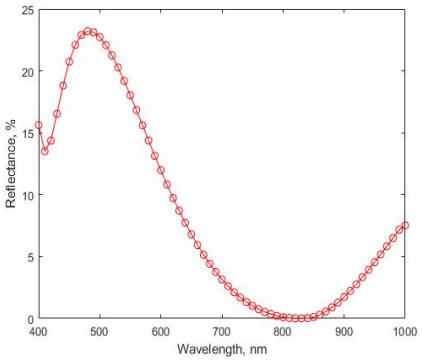
Antireflection of optical surfaces can be achieved by depositing a tailored thickness layer of a specific refractive index material on the surface [1]. Subwavelength diffraction gratings behave as uniform films of material and precisely realize the effective refractive index necessary for antireflection [2].

Methods

Rigorous Coupled Wave Analysis (RCWA) is a numerical method for computing reflectance of periodic optical structures [3]. Using it allows to determine geometry parameters of subwavelength diffraction gratings optimal for antireflection.

Results

RCWA implemented in MATLAB was used to estimate reflectance from the subwavelength grating in the visible spectral range. Geometry parameters were varied based on reflectance obtained from RCWA. Optimizable parameters of the grating were the fill fraction and grating pitch.



Reflectance of a silicon subwavelength 100 nm pitch diffraction grating optimized for 830 nm

Conclusions

The Rigorous Coupled Wave Analysis method was an effective tool for computing optimal structure parameters of an antireflective subwavelength diffraction grating operating in the optical wavelength range.

Acknowledgements

This work was supported by the Agency for Science, Innovation and Technology, Grant No. Biotech-02-014.

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ULTRAVIOLET LONG-LASTING LUMINESCENCE OF $CA_2AL_2SIO_7:PR^{3+}$

Dace Nilova, Andris Antuzevics, Guna Krieke

Institute of Solid State Physics, University of Latvia

Keywords
Ultraviolet light, persistent luminescence, calcium aluminosilicate

Actuality and aim
Materials with observable long-lasting luminescence in the ultraviolet (UV) range have a wide range of applications, such as disinfection, photocatalysis, biomedicine, therapies, etc. [1]. Understanding the formation of defects in the material is a prerequisite to determining the mechanism of persistent luminescence in the material and improving the properties of the material by introducing the necessary defects during the synthesis.

Methods
In the study, using the solid-state synthesis method, samples of $Ca_2Al_2SiO_7$ activated with different concentrations of Pr^{3+} were prepared and their luminescence properties were studied. X-ray diffraction (XRD), electron paramagnetic resonance (EPR), and luminescence spectroscopy methods were used to characterize the samples.

Results
$Ca_2Al_2SiO_7$ samples with Pr^{3+} concentrations in the range of 0-5 mol% were prepared. After irradiation with X-rays, persistent luminescence in the UV-C spectral range lasting more than 1 h is observed. Analysis of the EPR spectra shows that several paramagnetic centres are formed as a result of the irradiation. Thermal stimulation of the defects occurs in several stages in 25-250 °C range.

Conclusions
The optimal composition and synthesis conditions for the observation of intense UV-C persistent luminescence in the $Ca_2Al_2SiO_7:Pr^{3+}$ material were determined. Based on the obtained results about the formation and stability of the defects, a mechanism for long-lasting luminescence of the material is proposed.

Acknowledgements
Latvian Council of Science, project “Defect engineering of novel UV-C persistent phosphor materials”, project No. LZP-2021/1-0118 is gratefully acknowledged.

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DIELECTRIC PROPERTIES OF MIXED HALIDE PEROVSKITES

Robertas Grigalaitis [1], Sergejus Balčiūnas [1], Mantas Šimėnas [1], Martynas Kinka [1], Šarūnas Svirskas [1], Jūras Banys [1], Miroslaw Maczka [2]

[1.] Vilnius University, Faculty of Physics, Lithuania, [2.] Institute of Low Temperature and Structure Research, Polish Academy of Sciences

Keywords
Perovskites, solar cells, dielectric spectroscopy

Actuality and aim
Hybrid halide perovskites attract great attention due to their potential applications for efficient and inexpensive photovoltaic materials. The most known are methylammonium (MA) lead halides $MAPbX_3$ (X= I, Br, Cl) [1]. However, more stable and efficient solar cells are obtained by mixing MA with formamidinium (FA), ethylammonium (EA), dimethylammonium (DMA), etc.
It is well known that mixing may significantly perturb structure of resulting compound suppressing the long-range order and inducing frustrated phases. The dielectric permittivity studies seem to be especially informative analyzing such behaviour of such systems. However, a complete understanding of mixing effects on the dielectric permittivity dynamics and structural phase behavior is still absent.
Here we present a dielectric analysis of mix $MAPbBr_3$ systems (MA mixed with FA, EA and DMA) in a wide temperature and frequency range.

Methods
Dielectric spectroscopy experiments were performed in 20 Hz –1 GHz frequency range using HP4284A, Solartron Modulab XM MTS LCR meters and Agilent 8714ET vector network analyzer cooling samples at1 K/min rate.

Results
Experimental results show a similar behaviour for all mixed systems. With a low amount of substitute cations, we observe a slight shift of all phase transition temperatures toward lower temperatures. Higher amount of substitution results in a broadening and suppression of low temperature phase transition due to frustrated state.

Conclusions
Weak signatures of a dipolar glass phase are formed for the intermediate mixing levels.
The isotropic phase is effectively stabilized at low mixing level.

Acknowledgements
This project has been funded by the Research Council of Lithuania (LMTLT) (agreement No. S-MIP-19-4).

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ENHANCEMENT AND ORIGIN OF PHOTOCHROMISM IN BAMGSIO$_4$:FE

Haralds Ozols, Andris Antuzevics, Guna Krieke

Institute of Solid State Physics, University of Latvia

Keywords
Photochromism, EPR, diffuse reflectance spectroscopy

Actuality and aim
Organic compounds are mostly used as photochromic materials in industry due to their excellent contrast; however, they are not thermally resilient and have a limited number of cycles of color change. BaMgSi04:Fe is a material with good contrast and high repeatability of color change and is also thermally resilient. In this work, the origin of the photochromic effect in $BaMgSiO_4$:Fe is investigated.

Methods
Defects in $BaMgSiO_4$:Fe were studied with electron paramagnetic resonance (EPR) spectroscopy. Optical properties were studied with diffuse reflectance spectroscopy.

Results
Samples of $BaMgSiO_4$:Fe with Fe concentrations in range 0 – 5 mol% were synthesized in reducing H_2/Ar atmosphere. After irradiation of samples with UV light the samples turn to magenta color with light absorption peak at 523 nm. Measurements of $BaMgSiO_4$:Fe with EPR spectroscopy show an increase of signal corresponding to Fe^{3+} after irradiation with UV light.

Conclusions
Optimal concentration of Fe in $BaMgSiO_4$:Fe is found to be in the range 0.1 – 0.5 mol%. Results indicate that Fe ions act as electron donors. The contrast of color change, thermal resilience and the ability to be colored and bleached with widely available blue and green laser diodes show that $BaMgSiO_4$:Fe is a perspective inorganic photochromic material.

Acknowledgements
Financial support provided by Scientific Research Project for Students and Young Researchers “Origin and enhancement of photochromic effect in $BaMgSiO_4$:Fe” realized at the Institute of Solid State Physics, University of Latvia is greatly acknowledged.

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TRAPPING, RECOMBINATION AND GLOW MECHANISMS IN YAP:MN^{2+} CRYSTALS AS PROMISING TL/OSL DETECTORS

Yaroslav Zhydachevskyy [1], Hanka Przybylińska [1], Aneta Grochot [1], Vasyl Stasiv [1], Sergii Ubizskii [2], Marek Berkowski [1], Andrzej Suchocki [1]

[1.] Institute of Physics, Polish Academy of Sciences, Warsaw, Poland , [2.] Lviv Polytechnic National University, Lviv, Ukraine

Keywords
$YAlO_3$:Mn; EPR, thermoluminescence; trapping mechanisms

Actuality and aim
Mn^{2+}-doped $YAlO_3$ (YAP) is known as a perspective high-Z material applicable for thermoluminescent (TL) or optically stimulated luminescent (OSL) dosimetry of ionizing radiation (see [1] and references therein). In particular, the green-color emission from $Mn(Y)^{2+}$ ions occurring at the main TL peak at about 200 °C can be used for this purpose. This TL signal fades strongly at daylight (bleaching effect), therefore optical stimulation with visible light can be used for its readout [2].

Methods
The purpose of the present work was to perform a detailed EPR study of YAP:Mn^{2+} crystals and to correlate the obtained results with those of luminescence and optical absorption.

Results
It was found that only in yttrium-rich crystals Mn^{2+} ions undergo recharging to Mn^{3+} under ionizing irradiation, indicating that this process requires the availability of sufficiently deep electron traps. The presented results demonstrate, moreover, that Mn^{3+} + e --> Mn^{2+} recombination is not the most efficient excitation channel of the green $^4T_1 \rightarrow {}^6A_1$ emission of Mn^{2+}, possibly because of the huge energy difference between the recombination (>5.39 eV) and excitation (3 eV) energies. In contrast, energy transfer to Mn^{2+} proves to be dominant.

Conclusions
A general model of trapping and recombination mechanisms responsible for TL of YAP:Mn crystals above room temperature has been proposed. Beside Mn^{2+} ions and the defect-related electron and hole traps intrinsic to YAP lattice, the model includes also unintentional dopants like $Fe(Al)^{2+}$ acting as deep hole traps, as well as $Mn(Al)^{4+}$ and $Cr(Al)^{3+}$ ions acting both as deep hole and electron traps.

Acknowledgements
The work was supported by the Polish National Science Centre (project no. 2018/31/B/ST8/00774) and by the NATO SPS Project G5647.

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COMPUTER MODELLING OF WATER SPLITTING ON PEROVSKITE NANOPARTICLES

Leonid Rusevich [1], Eugene Kotomin [1], Guntars Zvejnieks [1], Yuri Mastrikov [1], Maksim Sokolov [1], Joachim Maier [2]

[1.] Institute of Solid State Physics, University of Latvia, Riga, Latvia, [2.] Max Planck Institute for Solid State Research, Stuttgart, Germany

Keywords
Water splitting, STO photocatalyst, band gap, DFT, faceted surfaces

Actuality and aim
Hydrogen production directly from water is the efficient source for green, environmentally friendly energy. Sunlight-driven water splitting is one of the most promising pollution-free strategies for production of hydrogen. The important task on this way is the improvement of photocatalytic materials properties.

Methods
Band engineering is one of the ways for development of the optimal photocatalytic material with both strong visible light absorption and high charge mobility. In this study, we performed ab initio unrestricted (open-shell) DFT calculations with the CRYSTAL17 computer code within the linear combination of atomic orbitals (LCAO) to investigate the structural and electronic properties of $SrTiO_3$ (STO) perovskite photocatalyst (band gap 3.25 eV) and to modify its electronic band structure by means of defects and impurities.

Results
We considered the bulk STO crystal and its (001) 2D slabs with different point defects (neutral and charged oxygen vacancies, nitrogen and aluminum substitutional atoms [1,2]). The electronic structure of defective systems was studied in details. Additionally, we simulated water molecule splitting on faceted STO surfaces on nanoparticles, which demonstrated recently high performance in hydrogen production. The optimal positions for water molecule dissociation were detected and analysed [3], proton formation and migration discussed.

Conclusions
Our computations demonstrate that introduction of N and Al dopants makes STO photocatalyst more efficient for sunlight-driven water splitting.

Acknowledgements
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EFFECTS OF SAMPLE PREPARATION METHODS ON LUMINESCENCE OF LITHIUM ORTHOSILICATE-LITHIUM METATITANATE CERAMIC PELLETS

Arturs Zarins [1], Mareks Senko [1], Madara Tomele [1], Aija Trimdale-Deksne [2], Aleksejs Zolotarjovs [3], Aleksandrs Dutovs [1], Juris Prikulis [1], Gunta Kizane [1]

[1.] Institute of Chemical Physics, University of Latvia, [2.] Faculty of Chemistry, University of Latvia, [3.] Institute of Solid State Physics, University of Latvia

Keywords
Lithium orthosilicate, Solid-state synthesis, Sol-gel, Luminescence.

Actuality and aim
Lithium orthosilicate is one of lithium containing compounds extensively studied for various application purposes, for example as tritium breeding ceramic for future thermonuclear fusion reactors due to high lithium density, high melting point, acceptable tritium release behaviour and good radiation stability [1]. To improve mechanical properties, lithium metatitanate is added to form biphasic lithium orthosilicate-lithium metatitanate ceramics which are regarded as the most promising tritium breeding material for ITER's test blanket modules [2].
Objective of this study is to analyse intrinsic point defects of lithium orthosilicate and lithium metatitanate, as well as biphasic pellets with content of lithium metatitanate ranging from 10 to 90 mol% prepared via solid-state and low-cost solution-based method, such as sol-gel (using nano-sized raw materials), using multiple luminescence methods.

Methods
To determine and characterise the crystalline phase composition of ceramic samples, powder X-ray diffractometry (p-XRD) was used. The luminescence was investigated using photoluminescence (PL), X-ray induced luminescence (XRL), and thermally stimulated luminescence (TSL) techniques.

Results
Results of p-XRD show, that obtained samples using low-cost methods contain desired crystalline phases.

Conclusions
The biphasic pellets have two PL bands at room temperature: (1) in blue-light region (430-460 nm) and (2) in red-light region (720-740 nm) related to intrinsic point defects in both components. The X-ray irradiated pellet samples have several signals in TSL glow curves between 350 K and 650 K indicating different trapping sites with various depths.

Acknowledgements
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REACTIVE E-BEAM EVAPORATION OF YTTRIUM:A SPECTRAL AND STRUCTURAL INVESTIGATION OF YTTRIUM OXIDE AND OXYHYDRIDE THIN FILM

Halil Arslan, Ilze Aulika, Anatolijs Sarakovskis, Liga Bikse, Georgijs Cikvaidze, Martins Zubkins, Juris Purans

Institute of Solid State Physics, University of Latvia

Keywords

photochromism, oxyhydride thin films, e-beam evaporation

Actuality and aim

In recent decade(s) there has been an increasing interest in the chromic materials because of the remarkable optoelectronic features they possess. Being the fact that the structural evaluation stays still uncertain, yttrium based oxyhydride thin films are the one of the most promising structures with photochromic behaviour [1,2]. In this research we aim to understand/construct the relation between crystal arrangements and spectroscopic and electrical characteristics of the yttrium, yttrium oxide and yttrium oxyhydride thin films.

Methods

E-beam evaporation, XRD, TEM, FT-IR, Spectroscopic ellipsometer, XPS, EXAFS.

Results

The findings of the absorption edge (K) of yttrium reveal that the oxidation state of Y in oxyhdride structure stays in the between the metallic yttrium and fully oxidized yttrium structure that corresponds to an unusual oxidation state. This result is in correspondence with the outcomes obtained from XPS, where the binding energy (Y 3d) shifts to the higher values depending on the chemical state of yttrium. The fully oxidized yttrium lattice vibrations at around 300, 380 and 550 cm^{-1} were detected by IR spectroscopy for yttrium oxide and yttrium oxyhydride thin films. The differences in the intensities and the widths of the vibration peaks indicates either the H atoms disturb the original cubic structure of sesquioxides and /or formation of new phases. This effect is visible either in the TEM images or on the X-ray diffractograms.

Conclusions

The findings from this study might enhance our understanding on the arrangements of H atoms in the host crystal structure which is directly related to the photochromic demeanour.

Acknowledgements

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1- DOI: 10.1063/1.4995081
2- DOI: 10.1103/PhysRevB.95.201301

OPTICAL PROPERTIES INVESTIGATION OF $K_2GD(PO_4)(WO_4)$:20%YB^{3+} AS A FUNCTION OF TM^{3+} CONCENTRATION

Julija Grigorjevaite [1], Arturas Katelnikovas [2]

[1.] Faculty of Chemistry and Geosciences, Vilnius University , [2.] Faculty of Chemistry and Geosciences, Vilnius University

Keywords
Upconversion, luminescence

Actuality and aim
One of the most serious worldwide problems is the counterfeiting of currency, goods, and important documents. One of the ways to prevent counterfeiting is down-conversion and up-conversion security pigments, where inorganic luminescent materials are used as security markers and security labels. Compounds with Tm^{3+} under near-UV and laser excitation emit light in the blue region of the visible spectrum.

Methods
$K_2Gd(PO_4)(WO_4)$:20%Yb^{3+} host matrix was synthesized by a solid-state reaction method. The stoichiometric amounts of high purity starting materials were weighed and mixed in agate mortar using acetone as a grinding media. The materials after the grinding were annealed at 873 K temperature. The Tm^{3+} concentration in $K_2Gd(PO_4)(WO_4)$:20%Yb^{3+} final compounds was 0.5 %, 1 %, 2 %, and 5 %.

Results
Upconversion emission spectra under 980 nm wavelength excitation show typical Tm^{3+} emission transitions. The most intensive emission lines were observed for $^3H_4 \rightarrow {}^3H_6$ transition at ca. 800 nm, and $^1D_2 \rightarrow {}^3F_4$, $^1G_4 \rightarrow {}^3H_6$ transitions at ca. 440 – 490 nm. A sample doped with 2% Tm^{3+} showed the strongest emission. Although the most intensive emission was observed at 800 nm, all samples appeared blue to the naked eye due to the low sensitivity of the human eye in the deep red spectral region.

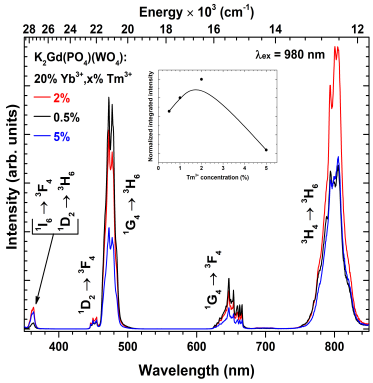


Fig. 1 Up-conversion emission spectra of $K_2Gd(PO_4)(WO_4)$:20%Yb^{3+} as a function of Tm^{3+} concentration.

Conclusions
The most intensive emission under 360 nm excitation was observed when Tm^{3+} concentration was 5 %, although the most intensive emission under 980 nm excitation was obtained for 2 % Tm^{3+} doped sample.

Acknowledgements
This research was funded by a grant (No. D-2018-0703 “Controlling the up-conversion emission by tuning band gap of the host matrix”) from the Research Council of Lithuania.

MECHANICAL STRESS VISUALIZATION OF ADDITIVELY BUILT (3D PRINTED) OBJECTS USING MECHANOLUMINESCENCE

Ernests Einbergs [1], Aleksejs Zolotarjovs [1], Donats Millers [1], Ivita Bite [1], Virgīnija Vītola [1], Agnese Spustaka [1], Gatis Tunēns [1], Aleksandr Arnautov [2]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Institute for Mechanics of Materials, University of Latvia

Keywords
mechanoluminescence, additive manufacturing, stress-strain analysis

Actuality and aim
3D printing is utilized for mechanical part manufacturing. Parts intended for demanding applications have to undergo one of the most important steps in complex part design: stress-strain analysis which tends to require significant know-how and is time-consuming [1].

Methods
In this study, we explored an innovative method for a spatial stress analysis of printed mechanical parts. A 3D printed photopolymer sample with $SrAl_2O_4$:Eu, Dy particle addition is tested and a method of data processing for spatial stress mapping is offered.

Results
The empirical stress distribution maps have proven to be in accordance with the calculated stress distribution and can therefore be further developed for technological applications offering a good addition for computational stress-strain analysis.

Conclusions
It opens the possibility for real-time evaluation of complex uneven forces on complex parts.

Acknowledgements
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OPTICAL PROPERTIES OF ZNMGO EPILAYERS GROWN ON SCALMGO$_4$ SUBSTRATE

Laima Trinkler [1], Ilze Aulika [1], Guna Krieke [1], Dace Nilova [1], Rihards Ruska [1], Jelena Butikova [1], Baiba Berzina [1], Liuwen Chang [2], Mitch Ming-Chi Chou [2]

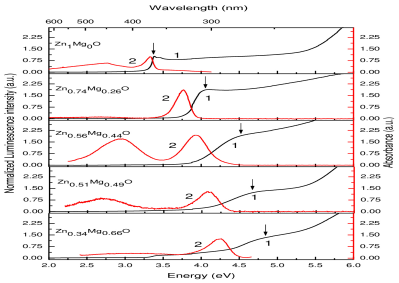
[1.] Institute of Solid State Physics, University of Latvia, [2.] Department of Materials and Optoelectronic Science, National Sun Yat-sen University, Kaohsiung , Taiwan

Keywords
Zn1-xMgxO thin films; optical spectroscopy

Actuality and aim
ZnO has attracted great interest as a material prospective for electronic and optoelectronic applications in the ultraviolet range due to the advantageous properties: direct wide band gap (3.37 eV at 4 K; 3.3 at RT) and large free exciton binding energy (60 meV). Even more possibilities for application in the deep UV region may be expected from ZnO compounds combining it with MgO. The task of the present study is to determine the band gap and other optical properties of wurtzite-type (WZ) $Zn_{1-x}Mg_xO$ epilayers depending on MgO concentration and to evaluate their applicability for deep UV sensors.

Methods
(WZ) $Zn_{1-x}Mg_xO$ (x= 0,..., 0.66) epilayers grown on SCAM substrate with the molecular beam epitaxy method were characterized using the methods of spectroscopic ellipsometry, optical absorption, and photoluminescence.

Results
Increase of MgO content in the $Zn_{1-x}Mg_xO$ compounds caused the blue shift of the band gap up to 4.35 eV at 10 K (4.32 eV at RT), an increase in exciton absorption and emission energy, and the blue shift of refractive index and extinction coefficient peak positions. The band edge emission was assigned to the luminescence of bound excitons. The increased values of Stokes shift and FWHM of exciton emission, thermal quenching activation energy, and Urbach tail in the absorption spectrum, were determined by the increased number of inhomogeneity-induced localization states with rising of MgO concentration.



Absorption (1) and photoluminescence (2) spectra of $Zn_{1-x}Mg_xO$ epilayers at 10 K.

Conclusions
The (WZ) $Zn_{1-x}Mg_xO$ epilayers grown on SCAM substrate demonstrated a tuned band gap in the UV region and could be recommended for application as UV light sensor materials, provided that some corrections in the production process were implemented to control the quality of the film structure [1].

Acknowledgements
M-ERA.NET project Nr. 1.1.1.5/ERANET/19/06 ZMOMUVS.

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NO DOPING? NO PROBLEM. LOW COST CARBAZOLE ENAMINES FOR EFFICIENT PEROVSKITE SOLAR CELLS.

Matas Steponaitis [1], Suer Zhou [2], Tadas Malinauskas [1], Vytautas Getautis [1], Henry J. Snaith [2]

[1.] Kaunas University of Technology, Lithuania, [2.] Department of Physics Clarendon Laboratory, University of Oxford, United Kingdom

Keywords
Enamines, hole transporting materials, low cost, perovskites, no doping

Actuality and aim
Perovskite solar cells deliver high efficiencies, but are often made from high-cost materials, such as the archetypical hole-conductor spiro-OMeTAD. In this work, new charge-transporting carbazole-based enamine molecules are reported. The new hole-conductors do not require chemical oxidation to reach high power conversion efficiencies (PCEs) when employed in negative-intrinsic-positive (n-i-p) perovskite solar cells, thus reducing the risk of moisture degrading the perovskite layer through the hydrophilicity of oxidizing additives that are typically used with conventional hole-conductors [1].

Methods
Synthesis, device fabrication, solar cell characterization,

Results
n-i-p devices made with new carbazole-based enamines achieved comparable PCE without doping, to those employing doped spiro-OMeTAD, and greatly enhanced stability under 85 °C thermal aging, maintaining 83 % of their peak efficiency after 1,000 hours, in contrast, the spiro-OMeTAD-based devices degrade to 26 % of the peak PCE within 24 hours.

Conclusions
As a result, we estimate that the overall manufacturing costs of hypothetical PV modules is reduced, making them feasible to compete with Silicon PV modules in terms of levelized cost of electricity.

Acknowledgements
The "Development of SemiTransparent Bifacial Thin Film Solar Cells for Innovative Applications" benefits from a € 1000000 grant from Iceland, Liechtenstein and Norway through the EEA Grants. The aim of the project is to develop materials for semi-transparent bifacial cost-effective solar cells, which operate in full and faint sunlight, as well as in backlit by snow-reflected conditions. Project contract with the Research
Council of Lithuania (LMTLT) No is S-BMT-21-1(LT08-2-LMT-K-01-003).

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OPTICAL PROPERTIES OF CU_2O SINGLE CRYSTALS AND THIN FILMS

Jevgenijs Gabrusenoks [1], Laima Trinkler [1], Dace Nilova [1], Rihards Ruska [1], Guna Krieke [1], Baiba Berzina [1], Liuwen Chang [2], Mitch Ming-Chi Chou [2]

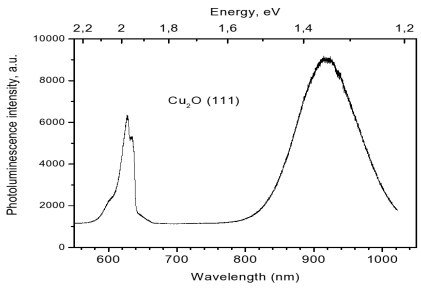
[1.] Institute of Solid State Physics, University of Latvia, [2.] National Sun Yat-sen University, Kaohsiung, Taiwan

Keywords
cuprous oxide, absorption, photoluminescence, exciton, vacancy

Actuality and aim
Cuprous oxide Cu_2O is used in a number of key enabling technologies, including thin film transistors, photovoltaics, water splitting, solar cells and others [1]. The task of the present study is characterizing Cu_2O single crystals and thin films by methods of optical spectroscopy.

Methods
Cu_2O single crystals were grown by the floating zone method and cut into (100) an (111) plates, while the Cu_2O thin films were produced by the electrodeposition method on crystalline Cu and polycrystalline Ag substrates. Materials were investigated by methods of optical absorption and photoluminescence (PL) in 10-300 K temperature range.

Results
The band gap of samples determined from the optical absorption using the Tauc method varies from 1.9 to 2.1 eV. PL of both single crystals and thin films has an emission spectra with an exciton band (620 nm) and defect bands (740, 820 and 920 nm) due to vacancies $v0^{2+}$, $v0^{+}$ and vCu, correspondingly. In single crystals the exciton emission band is clearly pronounced even at RT, while in thin films it is very small. At low temperature the 740 nm emission band is dominating. With temperature rise PL bands quench with different rate, and at RT only the 920 nm band is left. For the thin film samples the relative contribution of the defect subbands depends on spot of the sample surface.



PL spectrum of single crystal Cu_2O (100) under excitation 532 nm at RT.

Conclusions
Difference in spectral properties confirms the higher concentration of defects in thin films compared to single crystals of Cu_2O. Dominating of the 920 nm emission band at RT, testifies the presence of cupper vacancy, which is responsible for the p-type conductivity. Dependence of the spectra of the thin films on the PL signal detection spot speaks in favor of presence of domains with different crystallite orientations.

Acknowledgements
M-ERA.NET project Nr. 1.1.1.5/ERANET/19/06 ZMOMUVS.

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FLUORINE DOPED TIN OXIDE WORK FUNCTION MEASUREMENTS USING PHOTOELECTRON EMISSION YIELD SPECTROSCOPY

Andis Poļaks, Raitis Gržibovskis

Institute of Solid State Physics, University of Latvia

Keywords
Fluorine doped tin oxide, work function, photoelectron spectroscopy

Actuality and aim
Photoelectron yield spectroscopy (PYS) is a method to determine the ionization energy of a material. When studying electrically conductive metal oxides (ITO and FTO), the photoelectron yield spectrum shift was observed after repeated measurements. Similar shift has been described in previous studies with UPS and XPS methods [1-3]. The aim of this study was to find the possible reason for such shift and ways to avoid it.

Methods
PYS was used to determine the work function of two electrically conductive metal oxides - ITO and FTO. During the experiment, a sample is irradiated with changing photon energy UV radiation. From the spectrum, threshold energy is determined. The measurements were carried out in various conditions.

Results
FTO work function shift of 0.25 eV was observed by repeating the PYS measurements several times. While the measurements were carried out in vacuum, the variation of experiment conditions did not prevent the shift of work function. When the measurements were made in air, the shift in spectra was not observed.

Conclusions
1) While measuring the work function of FTO using the PYS, the photoelectron emission spectrum shifts were similar to those obtained by the UPS and XPS methods.
2) Measuring work function with PYS in the air prevents the shifts of spectra, and repeatable results are obtained since the measurement in the air does not affect the results.

Acknowledgements
The "Development of Semi‐Transparent Bifacial Thin Film Solar Cells for Innovative Applications" benefits from a € 1000000 grant from Iceland, Liechtenstein and Norway through the EEA Grants.

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LUMINESCENCE PROPERTIES AND ENERGY TRANSFER IN DY^{3+}/EU^{3+} AND TB^{3+}/EU^{3+} DOPED OXY FLUORIDE GLASSES AND GLASS-CERAMICS

Meldra Kemere, Uldis Rogulis

Institute of Solid State Physics, University of Latvia

Keywords
oxyfluoride glass-ceramics, photoluminescence, Eu^{3+}, Tb^{3+}, Dy^{3+}

Actuality and aim
Rare earth (RE) ions doped oxyfluoride glass-ceramics are perspective luminescent materials due to the high durability and low phonon energy they possess, and their optical properties have been investigated for use in sensors, lighting devices, etc [1]. Dy^{3+}/Eu^{3+} and Tb^{3+}/Eu^{3+} co-doped materials are widely used in optical devices, white light phosphors [2].

Methods
Oxyfluoride glasses with the compositions SiO_2-Al_2O_3-Na_2O-SrF_2 and SiO_2 Al_2O_3-CaO-CaF_2 doped with Tb^{3+}/Eu^{3+} ions and Dy^{3+}/Eu^{3+} ions (0-2 mol%) were synthesized via melt quenching method. The glasses were annealed at 650 °C - 750 °C temperature 1 to 4 hours to obtain glass-ceramics. Photoluminescence (PL) emission, excitation and decay measurements, and structure investigations (X-ray diffraction) were performed.

Results
In co-doped glasses, the PL intensity and decay times of Dy^{3+} and Tb^{3+} ions decreased with the increase of Eu3+ ions indicating the energy transfer between RE ions. In glass-ceramics with CaF_2 nanocrystallites, decay times decreased while with SrF_2 – increased.

Conclusions
PL measurements revealed that glass-ceramics containing SrF_2 show better incorporation of RE ions into the crystalline phase than samples containing CaF2 and it is associated with the increase of energy transfer between RE ions in SrF_2 containing samples. Heat treatment can be used to tune the luminescence colour of glass-ceramic samples.

Acknowledgements
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COLLECTIVE FUNCTIONALITY OF RESISTIVE SWITCHING IN NANOPARTICLE ASSEMBLIES

Blessing Adejube [1], Niko Carstens [1], Thomas Strunskus [1], Franz Faupel [1], Simon Brown [2], Alexander Vahl [1]

[1.] Institute for Materials Science – Chair for Multicomponent Materials, Faculty of Engineering, Kiel University, Germany, [2.] The MacDiarmid Institute for Advanced Materials and Nanotechnology, School of Physical and Chemical Sciences, Te Kura Mat ⊠u, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand

Keywords
Neuromorphic, Network, Nanoparticles Resistive Switching, Sputterring.

Actuality and aim

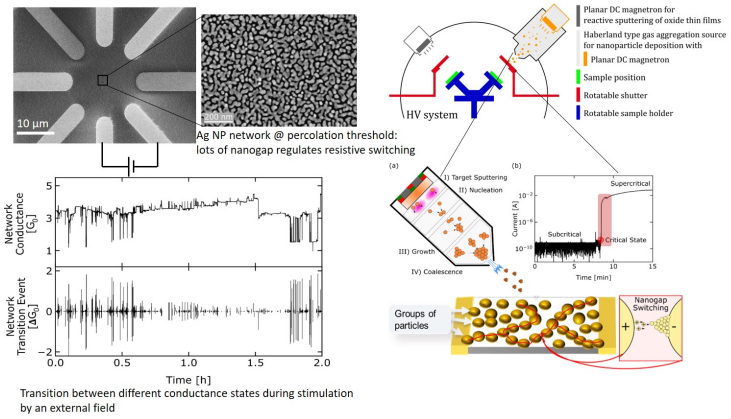
Intelligence, memory and learning are the results of neuronal system complexity and interaction between structure and function. Devices which can show both the temporal and topological features of neural networks like scale-free dynamics, long-range temporal correlation (LRTC) and self-organization, will be useful in designing a bio inspired computational hardware. The collective dynamics of complex nanoparticle (NP) networks poised at the percolation regime show resistive switching patterns which are similar in activity to neuronal dynamics. Thus are attractive for neuromorphic devices particularly those based on the concept of reservoir computing.

Methods

Ag NP networks are fabricated at percolation threshold using the gas aggregation source and SiO_xN_y capping layer is deposited by Reactive DC magnetron sputtering on to some of the Ag NP networks without breaking the vacuum. The evaluation criteria used are considered as characteristic for the operation regime of biological neuronal networks.

Results

The percolated nanoparticle networks exhibit a highly non-linear resistive switching activity which showed LRTC, scale-free dynamics and self-organisation. Interestingly, the collective dynamics of the network do not change significantly after incorporation of the dielectric matrix which means that the brain-like activities of the nanoparticle networks are retained.



Conclusions

The collective diffusive memristive switching and complex critical dynamics of the NP and without SiOxNy matrix are compared to showcase the application potential of NP as building blocks for resistive switching based neuromorphic devices.

Acknowledgements

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GA_2O_3 THIN FILMS DEPOSITED BY LIQUID METAL TARGET SPUTTERING

Edvards Strods [1], Martins Zubkins [1], Viktors Vibornijs [1], Edgars Butanovs [1], Liga Bikse [1], Juris Purans [1], Mikael Ottosson [2], Anders Hallen [3], Jevgenijs Gabrusenoks [4], Andris Azens [4]

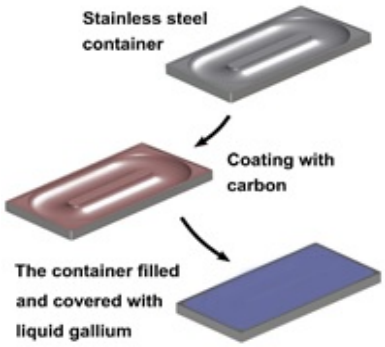
[1.] Institute of Solid State Physics, University of Latvia, [2.] Department of Chemistry, Ångström Laboratory, Sweden, [3.] KTH Electrum, Sweden, [4.] AGL Technologies SIA, Latvia

Keywords
Gallium oxide, thin films, reactive magnetron sputtering, liquid metal

Actuality and aim
Thin films of Ga_2O_3 are of technological interest due to their applications in wide bandgap electronic and optoelectronic devices [1,2]. Aim of the study is to demonstrate the possibility of deposition of stoichiometric Ga_2O_3 thin films by reactive DC magnetron sputtering form a liquid Ga metal target.

Methods
There is a variety of known methods used for Ga_2O_3 film deposition, including radio frequency (RF) magnetron sputtering from ceramic Ga_2O_3 targets [3]. In this study we report on amorphous and crystalline thin film coatings of Ga_2O_3 deposited by reactive direct current (DC) magnetron sputtering from liquid Gallium metal target onto fused (f-) quartz and c plane (c-) sapphire substrates with the substrate temperature varied from room (RT) to 800 °C.

Results
The deposition rate – up to 41 nm/min at room temperature on quartz and 5 nm/min at 800 °C on sapphire – is 2 to 5 times higher than the literature data for RF sputtering. At room temperature, the films are amorphous. Well defined XRD peaks of textured β–Ga_2O_3 start to appear at 500 °C substrate temperature. The films grown on c-sapphire at temperatures from 700 °C and up are epitaxial according to high resolution XRD. Electron microscopy images show dense and void-free films. The film optical properties are consistent with the literature data on Ga_2O_3 films produced by other methods of deposition.



Schematics of the target preparation

Conclusions
In this study we have demonstrated the possibility of deposition of stoichiometric Ga_2O_3 thin films by reactive DC magnetron sputtering form a liquid Ga metal target.

Acknowledgements
This study was funded by ERDF project No. 1.1.1.1/20/A/057 “Functional ultrawide bandgap gallium oxide and zinc gallate thin films and novel deposition technologies”.

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DIELECTRIC PROPERTIES OF $[NH_4][ZN(HCOO)_3]$ METAL FORMATE FRAMEWORK DOPED WITH ALKALI METALS.

Sergejus Balčiūnas [1], Barbora Škėlaitė [1], Mantas Šimėnas [1], Jūras Banys [1], Mirosław Mączka [2]

[1.] Faculty of Physics, Vilnius University, Sauletekio av. 3, LT-10257 Vilnius, Lithuania, [2.] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box-1410, PL-50-950 Wroclaw 2, Poland

Keywords
MOFs, ferroelectrics, multiferroic, formate, dielectric permittivity

Actuality and aim

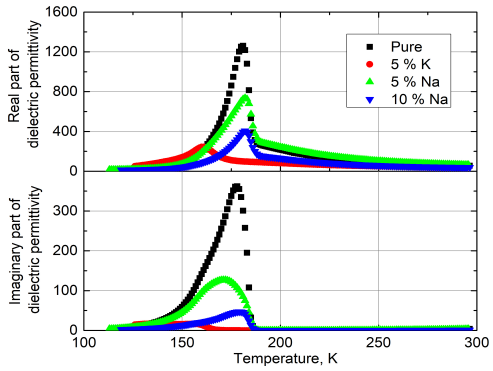
Recently a metal organic framework $[NH_4][Zn(HCOO)_3]$ has attracted interest of the scientific community. According to Guan-Cheng Xu et al. a paraelectric – ferroelectric phase transition (from P6322 to P63) was reported at 191 K temperature [1]. Furthermore, MOFs are likely candidates for magnetism, due to possibility to change metal centers, thus having a potential for single crystal multiferroic materials. Our initial studies revealed a tendency of alkali metals to diffuse into the structure of $[NH_4][Zn(HCOO)_3]$. Hence, the aim of this work is to investigate the effect on dielectric properties of K and Na impurities in the $[NH_4][Zn(HCOO)_3]$ crystal structure.

Methods

Dielectric measurements were performed in 130 – 300 K and 102 – 106 Hz frequency range using HP 4284A LCR meter. The crystals were cut in such a way that during electrical measurements the field in the crystal was parallel to the z axis. Experiments were performed at 1 K/min cooling/heating rates; temperature was measured with Keithley 2700 multimeter and RTD100 temperature sensor.

Results

In this poster presentation temperature (100-300K) and frequency (10 - 106 Hz) dependences of $[NH_4][Zn(HCOO)_3]$ will be presented. Temperature dependences at 1 MHz for pure and for different amount of impurities are shown in figure 1.



Temperature dependence of complex dielectric permittivity of $[NH_4][Zn(HCOO)_3]$ crystal.

Conclusions

Dielectric results show that with an increase of Na impurities the strength of the dielectric anomaly due to paraelectric – ferroelectric phase transition at 182 K decreases. Furthermore with 5 % K impurities this anomaly is less pronounced and shifts to lower temperature from 182 K to 160 K.

Acknowledgements

This project has received funding from the Research Council of Lithuania (LMTLT), agreement NO. S-MIP-22-73.

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MACRO- AND MICRO-SCALE INHOMOGENEITIES IN HEAVILY DOPED GADOLINIUM ALUMINUM GALLIUM GARNET SCINTILLATOR

Augustas Vaitkevičius [1], Mikas Iršėnas [1], Saulius Nargelas [1], Pavel Bohacek [2], Martin Nikl [2], Gintautas Tamulaitis [1]

[1.] Vilnius University, Lithuania, [2.] Institute of Physics of the Czech Academy of Sciences, Czech Republic

Keywords

Scintillator, Spatially-resolved photoluminescence, Confocal microscop

Actuality and aim

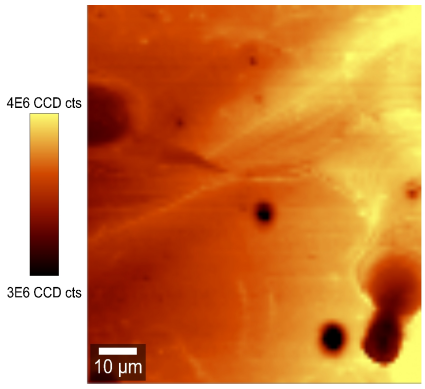
Novel scintillating materials with fast response are of increasing demand in the development of radiation detectors for medical imaging and high-luminosity high energy physics experiments. Multicomponent garnets are prospective scintillator host due to efficient transfer of excitation to activator ions, acceptance of heavy doping and efficiency in application of band gap engineering. However, the positive effect of heavy doping might be deteriorated by inhomogeneous distribution of the dopant. This work was aimed at the study of this effect.

Methods

The study was performed on a series of Czochralski-grown gadolinium aluminum gallium garnet (GAGG) single crystals doped with cerium and magnesium at different concentrations. Their photoluminescence properties were studied using WITec alpha300 S confocal microscope coupled with a spectrometer. Mappings of photoluminescence (PL) parameters with the spatial resolution of ~250 nm were obtained under excitation by a laser emitting at 442 nm to selectively excite Ce ions.

Results

Several types of microscopic defects, such as circular spots of increased or decreased PL intensity, were revealed and their evolution with increasing doping level was studied. The correlations between PL characteristics within the defects and in their surroundings were investigated. Radial dependence of macroscopic variations of PL properties in the crystal boule were also revealed.



Spatial distribution of photoluminescence intensity in GAGG:Ce,Mg single crystal.

Conclusions

Substitution of more than ~0.5 % of cations in GAGG lattice by Ce and Mg ions result in the formation of microscopic inhomogeneities of PL intensity. Dark and bright spots with the diameter of a few micrometers are formed. At lower doping and codoping levels of this scintillator, the luminescence spatial distribution is homogeneous.

RED AND INFRARED LUMINESCENCE IN CR^{3+} DOPED CALCIUM ALUMINATES WITH DIFFERENT CA/AL CONTENT

Pavels Rodionovs, Andris Antuzevics, Meldra Kemere, Uldis Rogulis, Anatolijs Sarakovskis

Institute of Solid State Physics, University of Latvia

Keywords
calcium aluminates, chromium, luminescence, electron paramagnetic resonance

Actuality and aim
Transition metal ions (Mn^{4+}, Cr^{3+}) doped optical materials emitting in the red and near-infrared range are used in applications for solid-state lighting, thermal sensors, bio-imaging, and others [1]. Calcium aluminate hosts are known as chemically stable and durable materials. In the present study, the photoluminescence properties and local structure of Cr^{3+} in calcium aluminates were investigated.

Methods
Cr^{3+}-doped polycrystalline calcium aluminate phases $Ca_3Al_2O_6$, $CaAl_2O_4$, $CaAl_4O7$, and $CaAl_{12}O_{19}$ were synthesized using the solid-state synthesis method. X-ray diffraction (XRD), photoluminescence (PL) and electron paramagnetic resonance (EPR) spectroscopy techniques were applied to characterize the samples.

Results
PL spectra with UV and visible excitation revealed both narrow and wide PL bands of Cr^{3+} in the red and near-infrared spectral ranges; their intensities were different for different phases. Cr^{3+}-related EPR signals were observed in all samples. Spin-Hamiltonian parameters were determined from EPR spectra simulations.

Conclusions
EPR spectra analysis revealed that the local structure of Cr^{3+} ions varies for calcium aluminates of different stoichiometry. $CaAl_{12}O_{19}$:Cr^{3+} showed the most intense PL both in the red and near-infrared range.

Acknowledgements
The financial support of ERDF project Nr.1.1.1.1/19/A/020 is greatly acknowledged.

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BROADBAND DIELECTRIC INVESTIGATION OF PEBA/UIO-66 MIXED MATRIX MEMBRANES

Martynas Kinka [1], Sergejus Balčiūnas [1], Robertas Grigalaitis [1], Gediminas Usevičius [1], Fa-Kuen Shieh [2], Andris Šutka [3]

[1.] Faculty of Physics, Vilnius University, Sauletekio av. 9, LT-10222 Vilnius, Lithuania , [2.] Department of Chemical Engineering, National Taiwan University, Taipei 10617, Taiwan, [3.] Institute of Materials and Surface Engineering, Faculty of Materials Science and Applied Chemistry, Riga Technical University, P. Valdena str. 3/7, Riga LV-1048, Latvia

Keywords
UIO-66, PEBA, dielectric spectroscopy

Actuality and aim
Recently UIO-66 metal-organic frameworks (MOFs) were identified as promising filler materials in mixed matrix membranes (MMM) for triboelectric nanogenerator (TENG) devices [1]. Such composites allow preservation of the original excellent properties and low preparation cost of polymers while the addition of functional fillers can effectively improve triboelectric properties of the membranes [2,3]. Energy harvesting is mainly affected by charge-inducing ability (surface properties) and charge-trapping capability (dielectric property) of triboelectric materials. In this study we have focused on broadband dielectric properties of polyether block amide (PEBA)/UIO-66 mixed matrix membranes aiming at investigation of dynamic processes in these composites.

Methods
Dielectric properties were investigated in 1 Hz – 1MHz frequency range using computer controlled ModuLab XM MTS impedance measurement system.

Results
PEBA-based MMM were prepared with 1, 2 and 5 wt% UIO-66 and UIO-66-NH2 concentrations. Dielectric properties were measured in 150 K – 360 K range during several heating-cooling cycles and compared with the response of vanilla PEBA sample. This allowed us to identify the influence of the filler/matrix interaction on the glass transition and melting/crystallization relaxations of polyether (PE) and polyamide (PA) segments.

Conclusions
Incorporation of UIO-66 crystallites increases glass transition temperature in PEBA matrix. On further heating relaxation process involving ionic charge carriers was observed, which was attributed to Maxwell-Wagner interfacial polarization resulting from the existence of well separated phases.

Acknowledgements
This project has received funding from the Research Council of Lithuania (LMTLT), agreement No S-LLT-21-2

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OPTICAL PROPERTIES OF HIGH-QUALITY ZNO / SIO_2 THIN FILMS GROWN BY MAGNETRON SPUTTERING

Mārtiņš Zubkins [1], Ramūnas Nedzinskas [1], Artūras Suchodolskis [2], Laima Trinkler [1], Juris Purāns [1]

[1.] Institute of Solid-State Physics, University of Latvia, Riga, Latvia, [2.] Center for Physical Sciences and Technology, Vilnius, Lithuania

Keywords
Energy band gap; Photoluminescence; absorption; excitonic transitions

Actuality and aim
Zinc oxide (ZnO) is an attractive semiconductor material for near-ultraviolet (UV) optoelectronic devices, owing to the wide energy band gap (3.37 eV) and high exciton binding energy (60 meV) at room temperature. However, it is still challenging to achieve a high-quality and stable ZnO thin films using fast, large-scale and industry-ready deposition techniques, such as magnetron sputtering [1].

Methods
In this work, ZnO thin films were grown on fused-quartz (SiO_2) substrate using a reactive DC magnetron sputtering method, aiming to derive the optimal deposition temperature. Optical properties of ZnO thin films, grown at 400, 550 and 750 ^oC temperature are investigated using room temperature optical absorption along with temperature- (3-300 K) and excitation- (80-700 kW/cm^2) dependent photoluminescence (PL) spectroscopy [2].

Results
Optical absorption allowed investigating the excitonic
absorption along with the band gap energy of ZnO at room temperature under Kubelka-Munk approximation. The PL features observed are attributed to different processes of carrier dynamics in the ZnO thin films studied. In particular, the sharp high-energy feature is due to near-band-edge optical emission from ZnO epitaxial layer, while low-energy PL bands are related to impurity-bound [3] and deep defect states.

Conclusions
Activation energy, Varshni parameters and exciton binding energy in ZnO thin films are estimated taking into account the optical band gap energy derived from absorption spectra. The optical parameters obtained are important feedback to adjust technological growth conditions.

Acknowledgements
The research was performed in a post-doc research project “Growth and characterisation of Ga_2O_3 and ZnMgO thin films for solar-blind ultraviolet applications”.

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OPTICAL SPECTROSCOPY OF ROCK-SALT $ZN_{(X)}MG_{(1-X)}O$ THIN FILMS WITH HIGH (UP TO 85%) ZN CONTENT

Monika Jokubauskaitė [1], Ramūnas Nedzinskas [1], Evelina Dudutienė [1], Artūras Suchodolskis [1], Laima Trinkler [2], Liuwen Chang [3], Mitch Chou [3]

[1.] Center for Physical Sciences and Technology, Vilnius, Lithuania, [2.] Institute of Solid-State Physics, University of Latvia, Riga, Latvia, [3.] Center of Crystal Research, National Sun Yat-sen University, Kaohsiung, Taiwan

Keywords
Photoluminescence; absorption; excitonic transitions

Actuality and aim
Zinc oxide (ZnO) and magnesium oxide (MgO) are hexagonal wurtzite (wz) and cubic rocksalt (rs) crystal structures, respectively. In a stable ternary compound of ZnMgO both Zn and Mg can be substituted by each other up to 40% [1]. ZnMgO solid alloy with a highly-tunable bandgap (from 3.3 eV to 7.8 eV) thus has a great potential for optoelectronics applications in the deep-UV spectral region [2]. However, it is difficult to grow purely either wurtzite or rocksalt ZnMgO epilayers exhibiting the bandgap energies between 4.3–5.4 eV [3]. Nevertheless, it was recently reported [4] that the use of lattice-matched MgO substrate provides ZnO solubility up to 85% sustaining single-phase rocksalt crystal structure.

Methods
In this work, room temperature absorption spectroscopy along with temperature- and excitation- dependent photoluminescence (PL) study of rs-ZnMgO epilayers grown on (100) MgO substrate by plasma-assisted molecular beam epitaxy is presented.

Results
Optical absorption allowed to determine bandgap anergy, while PL technique was used to explore interband excitonic and defect related optical transitions in rs-ZnMgO thin films with high Zn content. Moreover, activation energies provided insight into thermal quenching processes. Furthermore, it was found that thermal annealing favours in better optical yield, owing to the reduced density of threading dislocations in these highly-strained rs-ZnMgO thin films.

Conclusions
Optical methods used allowed investigating the fundamental parameters of ZnMgO epilayers. The optical parameters obtained are important feedback to adjust technological growth conditions.

Acknowledgements
The financial support of m-era.net project “ZnMgO materials with tunable band gap for solar-blind UV sensors” (ZMOMUVS) is acknowledged.

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OPTIMIZATION OF THE CHEMICAL COMPOSITION OF $CuInP_2S_6$ LAYERED CRYSTALS FOR ENERGY HARVESTING APPLICATIONS

Alexander Molnar, Henrietta Bán, David Gál, Andriy Haysak

Uzhhorod National University, Ukraine

Keywords
2D metal thiophosphate, $CuInP_2S_6$, chemical composition, energy harvesting

Actuality and aim
Among the materials based on which active elements of functional electronics devices can be created, the most promising are complex semiconductor chalcogenides on the state diagrams of which various phases are realized - ferroelectric, ferromagnetic, superionic, etc.
One of the most promising of them is $CuInP_2S_6$ layered crystals, in which ferroelectric ordering is observed even when the thickness decreases to 4 nm or less at room temperature [1].
We have been looking for ways to optimize the performance of these crystals to improve their performance for energy harvesting applications.

Methods
We have studied the effect of changing the chemical composition (deviation in stoichiometry) of 2D $CuInP_2S_6$ to increase the phase transition temperature and change their electrical properties (dielectric permittivity and bandgap). To this, $CuInP_2S_6$ crystals were grown with copper and indium deviations, and the temperature dependence of the permittivity, the intrinsic absorption edge, and the switching parameters were measured.

Results
As our studies have shown, an increase in the amount of indium by only 5 % in the composition of crystals leads to an increase in the phase transition temperature by 10 degrees, an increase in the band gap by 0.1 eV, and an increase in spontaneous polarization, which is very important for the use of these crystals as energy harvesters. In addition, an increase in the internal biasing electric field is observed, which makes it difficult to repolarize the sample; however, this feature also improves the practical prospects of crystals.

Conclusions
Increasing In in $CuInP_2S_6$ crystals improves their electrophysical properties for energy converters.

Acknowledgements
This report is based upon work partially supported by the ELTE Márton Áron College.

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COMPUTATIONAL STUDIES OF ATOMIC AND ELECTRONIC STRUCTURES OF "OXIDE CRYSTAL - OXIDE GLASS" INTERPHASES

Yuriy Hizhnyi [1], Vitaliy Chornii [1], Sergiy Nedilko [1], Andrzej Suchocki [2], Yaroslav Zhydachevskyy [2]

[1.] Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska st., Kyiv, Ukraine , [2.] Institute of Physics Polish Academy of Sciences, al. Lotników 32/46 Warsaw, Poland

Keywords
electronic structure, glass, molecular dynamics, interface, phosphate

Actuality and aim
Computational investigation of the atomic and electronic structures of interphases of technologically perspective composite materials is an actual problem of modern materials science [1-3].

Methods
Computational studies of the atomic and electronic structures of interphases in composites of different types were carried out by Materials Studio 2019 software package [4]. Two types of composites were considered: a) $KBi(MoO_4)_2$ crystal - phosphate-molybdate glass of K_2O-P_2O_5-MoO_3-Bi_2O_3 system; b) $K_2Eu(PO_4)(WO_4)$ crystal - phosphate-tungstate-vanadate glass of K_2O-P_2O_5-WO_3-VO_3 system. The atomic structures of interphase layers of composites were calculated by molecular dynamics methods using Amorphous Cell and Forcite programs. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method CASTEP.

Results
Obtained results on optimized geometries of interphases regions were used for calculations of the optical absorption spectra of particular oxyanionic molecular groups located in interphase regions by the TD-DFT method with use of Gaussian program.

Conclusions
Relationships between atomic and electronic structures of interphases layers and optical characteristics of studied composites were analyzed. The possibility of "engineering" the corresponding properties of a number of novel composite materials is discussed.

Acknowledgements
The calculations were performed using Bem supercomputer of Wroclaw Center for Networking and Supercomputing (grant no. 488).

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PHOTOELECTRICAL PROPERTIES OF NOVEL HOLE TRANSPORT MATERIALS FOR SEMI-TRANSPARENT SOLAR CELLS

Raitis Grzibovskis [1], Andis Polaks [1], Tadas Malinauskas [2], Aivars Vembris [1]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Kaunas University of Technology, Lithuania

Keywords
hole transport material, ionization energy, charge carrier mobility

Actuality and aim
The efficiency of solar cells is determined by several parameters such as charge carrier generation efficiency and generated charge carrier extraction from the solar cell. Charge carrier transport layers are introduced to help to extract holes and electrons from the cell. For such layers the energy level alignment and charge carrier mobility are important.
In this work, eight novel organic hole transport materials (HTMs) for Sb chalcogenide-based semi-transparent solar cells were studied. The energy level values as well as the charge carrier mobility were obtained.

Methods
The thin film samples were made from solutions by spin-coating. The photoelectron emission yield spectroscopy was used to determine the ionization energy level of HTMs. The gap between ionization energy level and electron affinity level was obtained from the intrinsic photoconductivity spectra of the materials. From this, the electron affinity level values were calculated.
The charge carrier mobility of the HTMs was obtained using the time of flight method.

Results
The ionization energy level values of the studied HTMs were between 4.80 and 5.10 eV. The hole mobility varied within one order of magnitude ranging from $1e^{-6}$ to $1e^{-5}$ cm^2/Vs and showed great influence on the molecule structure.

Conclusions
While the ionization energy level values of the studied HTMs were relatively close to each other, the hole mobility values varied greatly. This allows the selection of the most suitable materials based on their parameters.

Acknowledgements
The "Development of SemiTransparent Bifacial Thin Film Solar Cells for Innovative Applications" benefits from a € 1000000 grant from Iceland, Liechtenstein and Norway through the EEA Grants.

SYNTHESIS AND USE OF FUNCTIONALIZED GRAPHENE MATERIALS FOR ENERGY STORAGE

Roberts Olins [1], Peteris Lesnicenoks [1], Janis Kleperis [2], Ainars Knoks [2], Ingars Lukosevics [2]

[1.] Faculty of Materials Science and Applied Chemistry, Riga Technical University and Institute of Solid State Physics, University of Latvia , [2.] Institute of Solid State Physics, University of Latvia

Keywords
Graphene, N-doped, supercapacitors

Actuality and aim

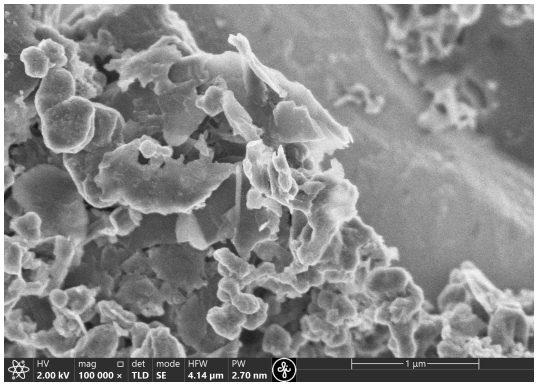
Due to a growing global demand for electricity in different devices therefore energy storage devices, supercapacitors have gained a large interest for commercial use. Graphene is a one atom thick carbon sheet with a very large surface area, high thermal and electrical conductivity. Functionalization of graphene is possible in many various ways and greatly improves upon it's capabilities - N-doping improves electrical conductivity. The aim of the study was to obtain and compare carbon materials that could be used as electrodes in supercapacitors for energy storage.

Methods

A method of electrochemical exfoliation in nitrogen rich electrolyes [2]–[4] was used to obtain graphene sheets. Graphene oxide was synthesized using a Modified Hummer's method for reference. The solution containing the obtained material were filtered through a 0,2µm filter and dried. The materials are later deposited on a Al foil sheets using Doctor Blade coating and electrodes were formed using a hydraulic press and inserted in a Swagelok cell with a micro fiberglass separator saturated with a LiPF6 electrolyte to create a supercapacitor.

Results

The obtained materials were characterized using SEM, XRD, XPS, Raman spectroscopy and potentiostatic measurements.



SEM image of graphene sheets on silicon

Conclusions

N-doped graphene sheets were obtain during electrochemical exfoliation process as well as graphene oxide and carbon quantum dots. Four supercapacitors were created from the obtain materials.

Acknowledgements

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THE APPEARANCE OF THE FLEXOELECTRIC COUPLING NEAR THE FERRIELECTRIC PHASE TRANSITION IN $CuInP_2S_6$ LAYERED CRYSTALS

Vitalii Liubachko, Anton Kohutych, Viacheslav Hryts, Konstantin Glukhov, Ruslan Yevych, Yulian Vysochanskii

Institute for Solid State Physics and Chemistry, Uzhhorod University, Pidgirna Str. 46, Uzhhorod, 88000, Ukraine

Keywords

$CuInP_2S_6$; acoustic phonons; Brillouin scattering; thermal conductivity

Actuality and aim

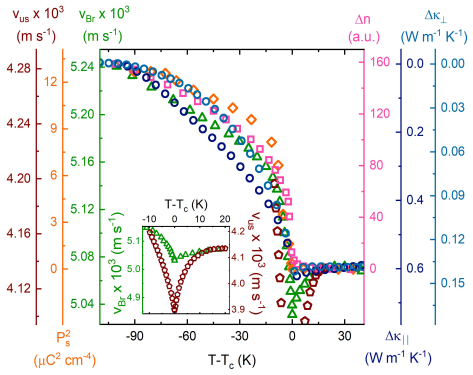
For the last decades, there is a huge interest in the development of different kinds of functional 2D materials. The possibility that they could support ferroelectric capabilities would open the door for bistable devices and functional electronics [1,2].

Methods

Layered $CuInP_2S_6$ single crystals were grown by a Bridgeman method. The acoustic phonons were calculated in the frame of DFT, their temperature dependence was studied by Brillouin spectroscopy as well as their thermal transport was analyzed.

Results

Comparison of anomalies (see in figure) of thermal conductivity deviations Δκ (circles) along and normally to a structural layer of $CuInP_2S_6$ crystal, with temperature behavior of the optical birefringence increment Δn (squares) [3], square of spontaneous polarization Ps^2 (rhombuses) [4], longitudinal ultrasound velocity vus normally to the layers (pentangles) [5], hypersound velocity vBr along the crystal layers (triangles) and a heat transferring acoustic phonons group velocity demonstrates evidence of acoustic softening in the paraelectric phase at cooling to the 1st order ferrielectric phase transition near Tc ≈ 315 K.



Anomalies in the properties of $CuInP_2S_6$ crystal near the ferrielectric phase transition

Conclusions

The Brillouin spectroscopy [6] and thermal conductivity studies [7] confirm earlier received ultrasound data [5] about unexpected elastic softening of $CuInP_2S_6$ compounds at the edge of stability of the paraelectric phase – at cooling to the first order transition into the ferrielectric phase. The observed effect at the high-temperature side of the order-disorder type phase transition can be related to the flexoelectric coupling of relaxational soft polar optical and acoustic branches. Such coupling can induce the inhomogeneously polarized state in the temperature region between paraelectric and ferrielectric phases.

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OPTIMIZATION OF KERATIN EXTRACTION METHOD FROM SHEEP WOOL

Vanda Voikiva [1], Elina Pajuste [1], Inga Jurgelane [2], Didzis Salnajs [1]

[1.] University of Latvia, Institute of chemical physics, [2.] Riga Technical University, Institute of General Chemical Engineering, Latvia

Keywords
Keratin, extraction, wool, feathers.

Actuality and aim
Keratin is main structural protein that is in hair, nails, feathers, horns and forms the outer layer of vertebrate skin [1]. For many decades keratin was known as protein with outstanding and remarkable properties, that was widely used in cosmetology and medicine, for hair, nail and skin renewal and improvement [2]. Recently great interest is attracted to it use in the field of biomaterials, keratin-based biomaterials that could be used for biomedical purposes.
Although, inefficient and complicated keratin extraction methods slow down the development of keratin applications in this field, and in general [2].

Methods
Bradford protein assay, SEM, FTIR.

Results
The analysis of the keratin extraction data obtained at different NaOH concentrations and temperatures shows a negative trend. A decrease in keratin yield for molecules larger than 12 kDa was observed with increasing reagent concentration and temperature.
The keratin extracts show a plaque-like structure, which is clearly visible in the keratin extracts of all methods. It is evident from the SEM images that an increase in temperature and reagent concentration also has a negative effect on the keratin structure. It becomes rougher and more uneven, and the number of cracks and holes increases significantly

Conclusions
By adjusting the keratin extraction parameters and lowering the process temperature, it is possible to significantly improve the keratin extraction yield.

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TUNGSTEN OXIDE, COPPER AND ZINC CONTAINING ANTI-MICROBIAL THIN FILM MAGNETRON SPUTTERING.

Viktors Vibornijs [1], Martins Zubkins [1], Anna Zajakina [2], Ksenija Korotkaja [2], Edvards Strods [1], Juris Purans [1]

[1.] Institute of Solid State Physics, University of Latvia, Kengaraga 8, LV-1063, Riga, Latvia , [2.] Latvian Biomedical Research and Study Centre (LBMC), Ratsupites 1, LV-1067, Riga, Latvia

Keywords
Anti-microbial, vacuum plasma, magnetron sputtering

Actuality and aim
Despite the recent decades significant progress in the fields of anti-microbial agents development, anti-microbial coatings are not well integrated in the industries related with pathogen spreading risks. New materials development and production process optimization remain to be the subject of science attention. Anti-microbial coatings biocidal effect is not selective on species or types of microorganisms and in case of effectiveness it affects patogens equally.

Methods
WO_{3-x}/Cu/WO_{3-x},WO_{3-x}:Cu,ZnO/Cu/ZnO and WO_{3-x}/Zn/WO_{3-x} composite thin films were prepared using magnetron sputtering technology. PET and soda-lime glass were used as substrate.

Results
Anti-microbial effects detected in most of the tested samples. Significant difference of efficiency evaluated between similar samples. Thin films were tested on 2 bacteria species and virus. Samples were more effective on gram-positive S.aureus bacteria. Colonia forming unit log reduction were 4 for all the WO_{3-x}/Cu/WO_{3-x} samples and 3 for ZnO/Cu/ZnO sample. Samples were partly effective on gram-negative E.coli with CFU log reduction from 1 to 2. Significant anti-viral efficiency was also detected on MS_2 virus, virus titer approximately reduced 100000 times. In case of poor WO_x, Cu, ZnO and Zn thin films significant anti-microbial efficiency were detected only for Cu. Cu sample efficiency were lower then WO_{3-x}/Cu/WO_{3-x} composite, but more efficient than Zn containings.

Conclusions
Vacuum plasma sputtering technology is effective tool for new anti-microbial coatings development due to possibility of coatings diverse property variation. Also relatively small changes un thin film coating properties can lead to changes in it's anti-microbial efficiency.

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ERAF project "Liela laukuma MABAV pārklājumi"

ASSESSING THE PERFORMANCE OF GRAPHENE-BASED GAS SENSORS IN AMBIENT AIR

Martin Lind, Valter Kiisk, Margus Kodu, Tea Avarmaa, Tauno Kahro, Raivo Jaaniso

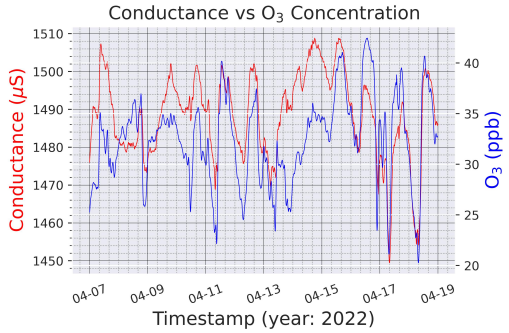
University of Tartu, Estonia

Keywords
Gas sensor, graphene, NO_2, O_3

Actuality and aim
Sensitive, miniature and low-power gas sensing elements are urgently needed for portable gas sensors, especially for monitoring common polluting gases, such as NO_2 and O_3. Besides achieving sufficient sensitivity and selectivity [1], one also needs to ensure long-term stability and correct sensor responses for environmental factors, such as temperature, humidity and air pressure.

Methods
We prepared CVD graphene-based chemiresistive sensors on Si/SiO_2 substrates. Graphene was functionalised with thin layers of various oxides using pulsed laser deposition. Electrical conductances of multiple such sensors were monitored for several weeks in ambient air. O_3 , NO_2 and tVOC concentrations were also monitored using reference sensors. Sensors' responses were analysed using linear regression.

Results
The responses of most sensors showed clear correlations with reference O_3 levels whereas some sensors suffered from notable drift over the measurement period. The "burn-in" time was usually a few days. Sensitivities to O_3 and NO_2, rate of sensor drift and correction factors to the environmental influences were quantified.



Sensor's reading (conductance) compared to commercial O3 sensor Aeroqual 500

Conclusions
It is possible to prepare graphene-based gas sensors that are reasonably sensitive and stable over several weeks to detect NO_2 and O_3 in ambient air with minimal interference of humidity.

Acknowledgements
This work has received funding from the European Union's Horizon 2020 research and innovation programme under Graphene Flagship grant agreement No 881603, from the Estonian Research Council (PRG1580), and from the European Regional Development Fund in the University of Tartu (Graduate School of Functional Materials and Technologies).

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LATTICE DYNAMICS AND RAMAN AND INFRARED REFLECTANCE SPECTRA OF $YALO_3$

Ciro Federico Tipaldi, Jevgēņijs Gabrusenoks, Georgijs Čikvaidze

Institute of Solid-State Physics University of Latvia

Keywords
phonon, lattice dynamics, perovskites, ab initio, Raman spectroscopy

Actuality and aim
A comprehensive study of the vibrational spectra and properties of yttrium aluminium oxide $YAlO_3$ (YAP). This study intends to supply additional Raman spectra accompanied by new results, and account for the lack of infrared reflectance spectra for YAP - a material with various uses in optoelectronics [1].

Methods
Ab initio and classical calculations in conjuction with polarized and low temperature Raman and infrared reflectance spectroscopy have been used for inquiry into the lattice dynamics of YAP of Pnma symmetry. X-ray diffraction analysis has been used for structural identification of samples.

Results
Complete polarized Raman spectra have been obtained in all polarizations, alongside with low-temperature spectra. Infrared reflectance spectra are presented. Phonon dispersion and DOS curves have been calculated theoretically and emerging properties obtained. Different DFT functionals have been compared in terms of their vibrational frequency prediction accuracy.

Conclusions
New vibrational maxima, predicted by calculations but not previously found in the literature [2, 3], have been identified. Infrared reflectance spectra will now be available for the present material. The results presented here help fill the picture for YAP regarding its lattice dynamics.

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ROLE OF NUCLEATION LAYER IN MOCVD GROWTH OF B-GA_2O_3 THIN FILMS

Gundars Strīķis, Lauris Dimitročenko, Edgars Butanovs, Līga Bikše, Juris Purāns

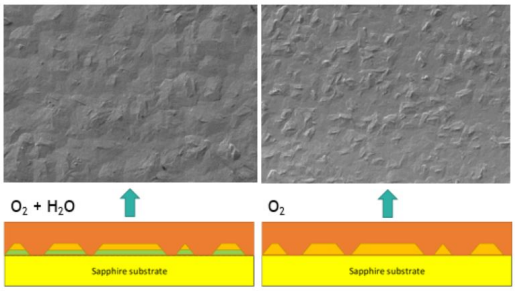
Institute of Solid State Physics, University of Latvia

Keywords
MOCVD, thin films, gallium oxide, nucleation layer

Actuality and aim
Gallium oxide (Ga_2O_3) is a promising wideband semiconductor material mainly due to its 4.8 eV wide bandgap. β-Ga_2O_3 epitaxial thin films have received increased attention in the last decade due to their potential applications in power electronics and optoelectronic devices. The use of nucleation layer during the deposition process has not been studied in previous works concerned with gallium oxide thin films.

Methods
β-Gallium oxide thin films were obtained on c-plane sapphire wafers using MOCVD (metalorganic chemical vapor deposition). Varied deposition parameters were used to determine optimal growth circumstances. Obtained thin films were studied by XRD, AFM, SEM, TEM.

Results
The thickness, deposition temperature and precursor ratio of the nucleation layer have significant impact on the quality of gallium oxide thin film. Water as oxygen source during the growth of the thin film causes large grain polycrystallic structure. Using oxygen gas as oxygen source during the growth of the thin film enables sub-micron grain structure with prevailing [201] crystallic orientation. The use of hydrogen as carrier gas enables desorption process.



Impact of varied nucleation layer growth parameters on the surface characteristics of β-Ga_2O_3 of

Conclusions
Ga_2O_3 epitaxial film obtained by the MOCVD method is the result of correctly selected growth regimes, their sequence and duration, as well as the control of the precursor concentration ratio used in the process.

Acknowledgements
The financial support of Latvian Council of Science project "Epitaxial Ga2O3 thin films as ultrawide bandgap topological transparent electrodes for ultraviolet optoelectronics" No. lzp-2020/1-0345 is greatly acknowledged.

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TIME-RESOLVED LUMINESCENCE STUDIES OF TERNARY HEXAFLUORIDES UNDER SYNCHROTRON RADIATION EXCITATION

Juhan Saaring, Sergey Omelkov, Alexander Vanetsev, Vitali Nagirnyi, Eduard Feldbach, Ivo Romet, Marco Kirm

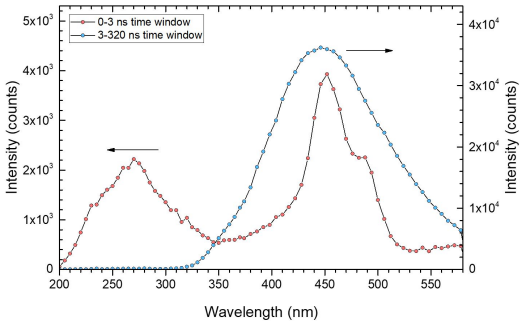
University of Tartu, Institute of Physics, Estonia

Keywords
scintillators, cross-luminescence, intraband luminescence

Actuality and aim
A wide range of applications in medicine, high-energy physics and elsewhere rely on high time resolution detection of ionizing radiation [1]. For example in positron emission tomography, a widely used medical imaging technique, the signal-to-noise ratio is dependent on the time resolution of the detection system. In this work, ternary hexafluorides with ultrafast cross- and intraband luminescence have been investigated to be used in novel scintillator materials.

Methods
Phase pure micropowders of several ternary hexafluorides were studied by time-resolved photoluminescence under VUV excitation at FinEstBeAMS and 10 keV X-ray pulses at the FemtoMAX beamline providing a superior time resolution of 32 ps in the MAX IV Laboratory (Lund, Sweden).

Results
As a result of these studies, nature of intrinsic emissions in ternary hexafluorides were revealed. Self-trapped exciton emissions with slow, microsecond range decay times were identified in all studied materials, but more importantly ultrafast emissions attributed to cross- and intraband luminescence emissions were observed from VUV to visible spectral range with decay times below 500 ps.



Emission spectra of BaGeF6 in two time windows, 0-3 ns and 3-320 ns.

Conclusions
This study demonstrates that ultrafast emissions in ternary hexafluorides from VUV to visible spectral range result from overlapping cross- and intraband luminescence. Properties of the ultrafast emissions indicate a high potential of intrinsic luminescence processes in the development of novel scintillator materials for specific fast timing applications.

Acknowledgements
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PREPARATION AND ELECTRIC CHARACTERIZATION OF LEAD-FREE FERROELECTRIC CERAMICS BASED ON SODIUM-POTASSIUM NIOBATE

Barbara Garbarz-Glos [1], Wojciech Bąk [1], Grzegorz Klimkowski [2], Maija Antonova [3]

[1.] Institute of Technology, Pedagogical University of Krakow, Poland, [2.] Institute of Technology, The Jan Grodek State Vocational Academy in Sanok, Poland, [3.] Institute of Solid State Physics, University of Latvia

Keywords
sintering, ferroelectric, niobates, electric properties

Actuality and aim
$(Na_{0.5}K_{0.5})NbO_3$ ceramics, as well as its modifications, are considered as one of the most perspective candidate to replace highly effective lead-based materials. The main advantage of these materials is high phase transition temperature (for NKN close to 670 K) in comparison with others lead-free materials with perovskite structure and other attractive electrical and piezoelectric properties. These properties offer the possibility of integrating NKN-materials as active elements of many electromechanical devices reducing the use of toxic lead-containing compounds in electronics.

Methods
The X-ray measurements were performed by means of on an X'Perrt PRO diffractometer. The investigations of microstructure, EDS and EPMA were carried out by means of Hitachi S4700 with microanalyses system Noran-Vantage. The electric properties were characterized using a Novocontrol System combined with Quatro Cryosystem for the temperature control and software package WinDeta.

Results
$(Na_{0.5}K_{0.5})NbO_3$ and $0.98(Na_{0.5}K_{0.5})Nb_{0.96}Sb_{0.04}O_3+0.02BaTiO_3$ were obtained by a solid state synthesis. The samples exhibit a crystalline perovskite structure, no formation of other phases was observed. The large difference in grain sizes is visible using admixtures. The character of the ac conductivity plots indicates a complex mechanism of electric charge transport.

Conclusions
Sb and BT modifications reduced the grain sizes and causes the shift of the Curie temperature towards lower temperatures of the investigated samples. It also reduces the maximum permittivity value and the paraelectric-ferroelectric phase transition is more diffuse.

Acknowledgements
Dr A.Łatkiewicz is acknowledged for SEM technical assistance

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ZNO-SCHIFF BASE COMPOSITES FOR OPTICAL DETECTION OF COPER IONS

Irina Tepliakova [1], Debleena Mandal [2], Dominika Jankowska [2], Viktoriia Fedorenko[3], Magdalena Barwiolek [2], Roman Viter [3]

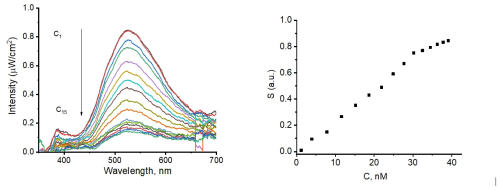
[1.] Odessa I.I. Mechnikov National University, Department of Experimental Physics, Ukraine, [2.] Nicolaus Copernicus University in Torun, Department of Chemistry, Poland, [3.] University of Latvia, Institute of Atomic Physics and Spectroscopy

Keywords
ZnO/Shiff base nanostructures, metal oxides, optical sensors

Actuality and aim
Optical sensors of metal ions today are an important promising direction in the environmental protection industry. The main requirements for the sensor are high sensitivity and selectivity.
Schiff bases are complex organic compounds with specific groups. The most important property of the Schiff bases is to host different metal ions. The affinity of the Schiff bases to different ions can be chemically tuned. Schiff bases require nanostructured template to improve sensitivity to the metal ions. ZnO nanostructures have advanced optical properties (room temperature photoluminescence at 378 and 530 nm). Optical emission of ZnO overlaps with optical absorption of Schiff bases, what can induce new optical properties and change electronic structure of Schiff bases.
In this work, we report on modifying of optical and sensitive properties of Schiff bases by integrating with ZnO nanostructures. Sensor tests to Cu^{2+} ions have been performed.

Methods
ZnO nanoparticles and Schiff base were added to chloroform and stirred for two days. The resulting compound was washed with methanol and dried in vacuum for 24 hours. Structure properties of the ZnO/Shiff base nanostructures have been investigated by SEM, FTIR, diffuse reflectance and photoluminescence (350-800 nm).

Results
The presence of the Schiff base of the structure led to a redistribution of emission bands in the photoluminescence spectrum of ZnO. The sensitivity of the resulting compound to copper ions was studied.



The dependence of photoluminescence on impurity concentration in solution and the sensitivity curve

Conclusions
ZnO/Schiff base nanostructure successfully synthesized, optical and structure properties were studied. The sensitivity of the obtained compounds to Cu^{2+} ions was found.

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IRIDIUM INCORPORATION DEFECTS IN GALLIUM OXIDE: AB-INITIO SIMULATIONS.

Aleksandrs Začinskis, Dmitry Bocharov, Alexander Platonenko, Anatoli Popov, Sergei Piskunov, Juris Purans

Institute of Solid State Physics, University of Latvia, 8 Kengaraga str., Riga LV-1063, Latvia

Keywords

First-principle calculations, gallium oxide, iridium impurities.

Actuality and aim

Recently, gallium oxide has become one of the most actively researched semiconductor materials today. The reason is its extremely promising electronic properties, such as wide bandgap, high theoretical breakdown field and high thermal and chemical stability. Due to these features, gallium oxide has potential applications in field-effect transistors, ultraviolet optoelectronics and other electronic devices. Bulk crystals of gallium oxide are usually grown by Czochralski (CZ) method in iridium crucible. In consequence, iridium is often present in CZ-grown gallium oxide crystals as an unintentional dopant. In this study, we present first-principles calculations of electronic properties of iridium doped gallium oxide in its monoclinic and corundum phases.

Methods

Ab-initio calculations were performed using CRYSTAL17[1] total energy code based on the linear combination of atomic orbitals method. Iridium incorporation defects were simulated by means of HSE06 hybrid exchange-correlation functional [2] within density functional theory and supercell approach.

Results

We report electronic band structure and density of states of iridium doped gallium oxide in its monoclinic and corundum phases, as well as formation energies and charge-state transition levels of iridium incorporation defects in all possible configurations.

Conclusions

Calculated properties let us better understand the implications of iridium doping in different phases of gallium oxide and propose practical applications of Ir doped Ga_2O_3.

Acknowledgements

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NEOPRENE AND ETHYLENE-OCTENE COPOLYMER COMPOSITES FOR TEMPERATURE SELF-REGULATING HEATING ELEMENTS

Astrida Berzina, Igors Klemenoks, Maris Knite

Riga Technical University, Latvia; Institute of Technical Physics

Keywords
Positive temperature coefficient of resistivity (PTC) self-regulating heating

Actuality and aim
Self-regulating heating materials could be a new standard for maintaining body warmth in cold outdoor conditions. Flexible heating elements without incorporated temperature controlling elements would be desirable in fields like winter clothes or diving suites. The aim of this study is to investigate possible polymer composite materials for PTC effect which enables self-regulating features – electrical resistance increases with temperature increase [1] as well as to determine the temperature range of self-regulating.

Methods
Ethylene octene copolymer (EOC) and neoprene (NP) samples with carbon black (CB) as electro-conductive filler were prepared. The CB amount varied from 10 phr to 30 phr. The electrical resistance dependence on temperature while heating externally 30 °C to 60 °C and the temperature, resistance and current dependence on applied voltage (5 V to 30 V) was determined by Joule heating internally.

Results
Both composites show PTC effect while heating externally. But while heating internally, EOC-CB composites still show PTC, but NP-CB samples exhibit the complete opposite effect – NTC – the resistance decreased with increased temperature. Human body heating elements need around 50-60 °C heating capabilities. The closest equilibrium temperature for EOC samples was ~60 °C for samples with 25 phr and 0,3 V/mm applied voltage, but NP-CB samples at the same applied voltage of 0,3 V/mm showed comparable temperature only for 30 phr samples – 53 °C.

Conclusions
EOC-CB samples can function as a self-regulating heating element. To achieve temperatures which would be usable as a human body heater of around 50-60 °C, the material needs at least 25 phr CB and 0,3 V/mm applied voltage.

Acknowledgements
The financial support of RTU Doctoral Research Scholarship is greatly acknowledged.

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LUMINESCENCE AND ELECTRON PARAMAGNETIC RESONANCE OF CARBON-DOPED SILICA GLASS

Madara Leimane [1], Ivita Bite [1], Anders Hallén [2], Linards Skuja [1]

[1.] Institute of Solid State Physics, University of Latvia, [2.] KTH Sweden

Keywords
Silica glass, sol-gel, ion-implantation, carbon doping, luminescence, EPR

Actuality and aim
High purity silica glass is material of choice in optical fibers, radiation-resistant and UV optics. Its synthesis increasingly shifts from using $SiCl_4$ precursor to silicon-organic compounds, which may introduce C impurities. While large C concentrations in SiO_2 (oxycarbide glasses) have been much studied, the properties of low-concentrations of C are less known. The aim of the present work is to obtain the photoluminescence (PL) and electron paramagnetic resonance (EPR) properties of C impurities in silica.

Methods
Carbon was introduced in silica samples as a by-product of glass sol-gel synthesis from silicon-organic precursor (TEOS) or by implantation of C^+ ions in dry synthetic silica glass (50 keV, 1×10^{15} – 3×10^{16} ions/cm^2). To assess the contribution of glass network damage, samples implanted by inert Ne+ ions were also prepared. The optical absorption, PL and EPR spectra were measured.

Results
All ion-implanted samples showed PL due to intrinsic defects: divalent Si (SiODC) and nonbridging oxygen (NBOHC). In C-implanted samples an additional PL band at 2.15 eV (excitation band at 4.95 eV) appeared. Similar green PL band emerged in sol-gel glass after annealing at 1200 C. EPR spectra of all samples showed signals at g=2.0008 due to Si E'-centers. C-implanted samples gave an additional signal at g=2.0024, which by comparison of data on centers on SiO_2 surfaces [1] can be tentatively assigned to Si-coordinated carbon radical $(Si)^{3-}C\bullet$ in silica glass.

Conclusions
C impurities in silica give rise to green PL band at 2.15 eV. One of the possible structural forms of C in silica is Si_3C cluster, where each Si atom is bonded via 3 oxygens to silica glass network.

Acknowledgements
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THE ORBITAL NATURE OF ELECTRON HOLES IN $BAFEO_{3-\Delta}$ AND IMPLICATIONS FOR DEFECT CHEMISTRY

Maximilian F. Hoedl, Rotraut Merkle, Eugene Kotomin, Joachim Maier

Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Keywords
Defect Chemistry, Electronic Structure, Protonic Ceramic Fuel Cells

Actuality and aim
BaFeO3–δ belongs to the class of mixed electronic-ionic conductors with contributions from electron holes, oxygen vacancies and hydrogen ion (proton) interstitials. The coexistence of multiple charge carrier types gives rise to unique functional properties, which are particularly useful in fuel- or electrolyzer-cells. Here we provide a chemically intuitive description of the electronic structure of $BaFeO_{3-\delta}$ and elucidate why electronic and ionic charge carrier concentrations are strongly correlated.

Methods
Density functional theory (DFT) calculations using plane wave-based functions with a posteriori projection onto an auxiliary basis set of local atomic orbitals.

Results
The calculations reveal $BaFeO_{3-\delta}$ to be a negative charge transfer material with a dominating d5L (L = ligand hole) configuration. A chemical bonding analysis shows that the ligand holes are partially delocalized in pdσ-bonds, with an approximate 80 % share at the oxygen ions. Consequently, oxygen ions are the redox-active species. This manifests in systematic variations of defect formation energies as a function of hole concentration, if oxygen ions are involved in these reactions. Specifically, we find that (i) oxygen vacancy formation energies increase with decreasing hole concentration, and (ii), proton uptake becomes more favorable with decreasing hole concentration.

Conclusions
Electron holes in $BaFeO_{3-\delta}$ have a dominant oxygen (ligand) character which has direct implications for the defect chemistry: The reaction energies of both oxygen vacancy formation and proton uptake vary systematically with hole concentration.

Acknowledgements
We are grateful for the computational resources by the HLRS DEFTD project (12939)

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OPTICAL WRITING IN THE STRUCTURE OF NEGATIVE SU8 PHOTORESIST USING UP-CONVERSION LUMINESCENCE OF YB^{3+} AND TM^{3+} ACTIVATED NANO-PARTICLES

Ernests Tropiņš, Jūlija Perveņecka, Kaspars Vītols, Viesturs Vīksna, Jānis Teterovskis, Jurģis Grūbe , Aivars Vembris, Jeļena Butikova, Guna Krieķe, Māris Spriņģis

Institute of Solid State Physics, University of Latvia

Keywords
photolithography, up-conversion luminescence, organic chromophores

Actuality and aim
Nowadays a topical problem in photolithography is the creation of structures containing organic chromophores, because of their high absorption at wave lengths commonly used in photolithography. Our goal is to develop a method for creating such structures using up-conversion luminescence nano-particles.

Methods
Traditionally exposition is done with UV radiation through the samples surface, but this is limited by the thickness of the photosensitive layer. In thick samples most of the radiation is absorbed in the upper layers, which results in unexposed deeper layers. Usually this can be solved by increasing the intensity of the radiation used, but that cannot be done if there are organic chromophores added to the photoresist, because the high intensity radiation destroys the organic molecules.
Our proposed solution is adding nano-particles, in which up-conversion luminescence occurs, to the photoresist so a radiation at a wave length that does not interact with organic chromophores can be used to initiate exposition within the volume of the photoresist.

Results
A method for creating optical writing using up-conversion luminescence in photoresist/nano-particle has been developed, viability of photoresist/organic chromophore/nano-particle system has been tested. We still have to develop a method for creating consistent optical writing in such system.

Conclusions
There are perspective applications for organic light emitting microstructures and our work will make the creation of such structures easier.

Acknowledgements
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CHEMIRESISTIVE GAS SENSORS BASED ON THE CORE-SHELL NANOCOMPOSITES OF THE CONDUCTING POLYMER

Nikolay Ogurtsov [1], Andrii Mamykin [2], Oleksandr Kukla [2], Alexey Pavluchenko [2], Jean-Luc Wojkiewicz [3], Alexander Pud [1]

[1.] V. P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine , [2.] V. E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, [3.] IMT Lille Douai, Institut Mines-Télécom, Univ Lille, Centre for Environment and Energy, France

Keywords
sensor, conducting polymer; carbon nanotubes, poly(vinylidene fluoride)

Actuality and aim
Despite many works devoted to gas sensing application of conducting polymers (CP) and their nanocomposites (NC), there is still incomplete understanding the mechanism of changing their resistance and sensitivity of sensors based on such materials, in particular in the case of physical adsorption of volatile organic compounds (VOC) [1]. Therefore, we studied sensing behaviors NCs with different cores of conducting MWCNTs or dielectric PVDF particles and CP shells.

Methods
Chemical oxidative polymerization, TEM and SEM, DC conductivity, sensory setup described earlier [2].

Results
NCs were prepared with cores of submicron PVDF particles or MWCNT and irregular or uniform poly(3-methylthiophene) (P3MT) shells, respectively.
The dependence of the sensory response (SR) to VOC on the loading of the P3MT in two NC series is opposite. The higher P3MT content in MWCNT/P3MT NCs the stronger responses are observed. On the contrary, the higher P3MT content in the PVDF/P3MT NCs the weaker responses are observed.
SR of composites of both types follow the same patterns:
$k \approx \varphi_i + b_i (\varphi_i - x_M)$,
where k is the sensor sensitivity, φ_i is the work function of the NCi, x_M is the electronegativity of VOC molecule, b_i is a constant. The equation is valid if $(\varphi_i \pm x_M)$ does not exceed 0.3 eV.
SR dependences of the NCs on Hansen solubility parameters revealed that that swelling in VOC has a significant effect on PVDF-based NCs sensitivity.

Conclusions
Sensitivity of chemiresistive gas sensors based on the core-shell CP NCs can be qualitatively predicted for different VOCs physically adsorbing on the CP surface. We experimentally determined limits of applicability of the developed approach.

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UV-CURABLE POLYMER MATERIALS FOR COATING AND ON-SITE REPAIR OF PHOTOVOLTAIC MODULES OF SOLAR CELLS

Tetiana Samoilenko, Natalia Yarova, Larysa Yashchenko, Oleksandr Brovko

Institute of Macromolecular Chemistry of the NAS of Ukraine

Keywords
Transparent coatings, epoxy polymer, sunlight UV-curing, photovoltaic module

Actuality and aim
Taking into account current ecological concern, the widespread application of solar energy is undoubtedly essential. Photovoltaic (PV) modules of solar collectors are now covered with glass, which makes them both heavy and brittle [1]. With the use of transparent polymer materials it is possible to overcome these drawbacks of solar cells and to prolong their expiration time. So, the aim of the research given is to estimate the efficiency of PV modules covered with epoxy coatings and to compare it with the one of glass laminated modules.

Methods
Easy to handle solvent-free epoxy formulation with triarylsulphonium hexafluorophosphate salts as a photoinitiator has long-term viability under storage in dark. After application on the surface of PV module it was irradiated by UV-lamp or sunlight. The parameters of PV modules were measured before and after sealing with polymer coating and glass laminate.

Results
The use of polymer coatings for solar cells protection faces the problem of decrease in the efficiency of PV modules. However, the results of investigations presented in the table show that the efficiency of PV modules covered with epoxy coating is even 26 % higher than the one of glass laminated module.
Moreover, as it was found before [2], given coatings have high optical transparency, adhesion, mechanical properties, weather resistance, and wide working temperature range.
The application of sunlight induced polymerization also allows on-site repair of existent coatings that are damaged. With the addition of photosensitizers it is possible to cure materials even at cloudy winter weather [3].

Sample	Open circuit voltage, V	Short circuit current, A	Efficiency, %	Change in efficiency, %
Uncovered PV module	1.22	2.9	18.90	-
Glass laminated PV module	1.10	2.8	16.45	-12.9
PV module with polymer coating	1.25	3.2	21.37	+13.0

The parameters of PV modules

Conclusions
Altogether, obtained polymer materials are shown to be effective protective coatings of photovoltaic modules and may be suggested for their covering or repair.

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NEW LASER MATERIALS BASED ON POLYURETHANE WITH CHEMICALLY BONDED POLYMETHINE DYE

Lyudmila Kosyanchuk[1], Tamara Bezrodna[2], Volodymyr Bezrodny[2], Oksana Antonenko[1], Alexander Ishchenko [3], Anatoliy Negriyko [2]

[1.] Institute of Macromolecular Chemistry NAS of Ukraine, 48 Kharkivske shose, Kyiv 02160, Ukraine, [2.] Institute of Physics NAS of Ukraine, 46 Nauki av., Kyiv 03028, Ukraine, [3.] 3Institute of Organic Chemistry NAS of Ukraine, 5 Murmanska st., Kyiv 02660, Ukraine

Keywords
polyurethane, polymethine dye, covalent binding, IR-spectroscopy

Actuality and aim
Interest in polyurethanes (PU) as matrices for the solid-state dye lasers is caused by their high polarity, resulted in greater solvation of dye molecules and prevention the formation of their associates. The covalent bonding between the dye molecules and polymer chains promotes more uniform distribution in the polymer bulk and provides additional channels for dissipation of the light energy not converted into radiation. Therefore, the development of functional materials on colored PU, in which organic dyes are covalently bonded to the matrix, is of an actual task. To expand the range of such dyes, unique converters of light energy, polymethine dyes (PD) were studied.

Methods
IR-spectroscopy, visible spectroscopy.

Results
The IR spectral analysis for the product of interaction between the indolenine salt, corresponding to the end heterocyclic fragment of PD, and phenyl isocyanate, initial salt and phenyl isocyanate shows the formation of urethane. This allows suggesting that PD are built into the PU chain. Covalent binding between the PD and PU results in higher rigidity of the chromophore structure by reducing the conformational mobility of the dye molecule, which increases the optical density ratio for the long-wavelength and short-wavelength absorption peaks.

Conclusions
The spectral-luminescent properties of the PD can be optimized by covalent binding to the cross-linked PU, compared to its mechanical doping in the polymer bulk. It is significant that the proposed method provides possibility to increase the absorption cross-section and fluorescence quantum yield even at high concentrations of dyes. This is of high importance for the development of new dye-doped polymers, in particular for active laser media [1].

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STABILIZED CARBON NANOTUBE/POLYPYRROLE NANOCOMPOSITE FOR VOC DETECTION

Nataliia Davydenko [1], Iryna Myronyuk [1], Nathalie Redon [2], Jean-Luc Wojkiewicz [2], Yuriy Noskov [1], Alexander Pud [1]

[1.] V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Sciences of Ukraine, 50 Kharkivske Shose, 02160, Kyiv, Ukraine, [2.] IMT Lille Douai, Institut Mines-Télécom, Univ Lille, Centre for Environment and Energy F-59000 Lille, France

Keywords
Carbon nanotubes, polypyrrole, nanocomposite, chemoresistor, sensor

Actuality and aim
Nanocomposites of conducting polymers (CP) with carbon nanotubes (CNT) are highly sensitive to volatile organic compounds (VOC) [1]. However, their using in sensors is limited by aggregation in dispersions needed to precipitate such materials on electrodes of chemoresistive gas sensors. While pure CNT aggregation can be regulated by surfactants or clays [2] there is a gap in information how to stabilize dispersions of the nanocomposites. Our work is aimed to fill this gap on the example of CNT nanocomposite with important CP polypyrrole (PPy).

Methods
FTIR, TEM, thermogravimetry (TG), conductivity and gas sensing

Results
The synthesized CNT/PPy nanocomposite has core-shell morphology. Specific interactions between PPy and CNT affect doping degree of PPy, conductivity and sensory properties of the nanocomposite. The nanocomposite sensitivity to VOC is enhanced due to addition of surfactants sodium dodecyl sulfate (SDS) or sodium dodecylbenzene sulfonate (SDBS) and smectite clay in its water dispersion. In particular, without additives the sensor demonstrates low responses. The highest response enhancement (fourfold) was obtained in case of using the clay additive to the PPy/CNT dispersion while in cases of SDS and SDBS there were around two times magnification. The results indicate improved state of the nanocomposite network on the electrodes of transducer due to presence of the additives. However, the level of this improvement depends of nature and quantity of the additive.

Conclusions
We synthesized new CNT/PPy nanocomposite and suggested ways to improve its properties. Sensor platform based on this nanomaterial with the surfactants or smectic clay shows enhanced responses 2-4 times higher than the initial nanocomposite without additives.

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THE EFFECT OF POLYANILINE CONTENT ON THE GAS SENSING PROPERTIES OF CONDUCTING HALLOYSITE–POLYANILINE NANOCOMPOSITES

Iryna Myroniuk [1], Yuriy Noskov [1], Nikolay Ogurtsov [1], Valery Bliznyuk [2], Alexander Pud [1]

[1.] V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, National Academy of Sciences of Ukraine, 50 Kharkivske Shose, Kyiv 02160, Ukraine, [2.] Environmental Engineering and Earth Sciences, Clemson University, Clemson, SC 29634, USA

Keywords
Halloysite nanotubes. Polyaniline. Nanocomposites. Properties. Gas sensing.

Actuality and aim
A growing anthropogenic air pollution demands using new effective gas sensors for environmental monitoring. To respond this challenge, we synthesized new nanocomposites based on natural tubular nanomaterial halloysite (HNT) with high specific surface and functional conducting polymer polyaniline (PANI) [1,2].

Methods
TEM, FTIR- and UV–Vis spectroscopy, thermogravimetric analysis (TGA), DC conductivity and chemoresistive sensor measurements.

Results
The nanocomposites HNT/PANI with different contents of the conducting polymer PANI doped with p-toluenesulfonic acid (TSA) were synthesized. TEM images of the nanocomposites demonstrate their core-shell morphology with HNT core and PANI shell with thickness increasing with content of PANI. Molecular structure and composition of the nanocomposites were characterized by FTIR and UV–Vis spectroscopy measurements. TGA showed that thermostability of the samples significantly enhanced at low PANI-TSA contents in the nanocomposites. Specific interactions between PANI-TSA and HNT components surface resulted in some improved properties of former as compared with that of the pure PANI-TSA. In particular, the best thermostability and sensing behavior were found for the nanocomposites with the lowest contents of the doped PANI (≤ 15.8 wt.%). The highest sensitivity to ammonia, acetone and isopropanol was observed for the nanocomposite with 7.0 wt.% of PANI.

Conclusions
The new sensing nanocomposites HNT/PANI-TSA have been synthesized These nanocomposites reveal the strong dependence of their morphology, molecular structure, conductivity, thermostability and sensor behaviour on the contents of the doped PANI. The best properties are observed at lowest contents of the doped PANI component (≤ 15.8 wt.%).

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STRUCTURE AND TRANSPORT PARAMETERS OF BINARY POLYACRYLIC ACID / POLYSILOXANE HYBRIDS

Olga Slisenko, Vira Budzinska, Iryna Bei

Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine

Keywords
hydrogel, polyacrylic acid, polysiloxane, swelling kinetics

Actuality and aim
Deficiency of water is considered as one of the major challenges in a great number of countries. Under such condition, hydrogels can be used as an alternative way which helps to reduce the problem of water scarcity for agricultural applications.
The aim of the study was development of organic/inorganic hydrogels based on sodium salt of polyacrylic acid (PAANa) and poly-N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (PAPTMS) with improved swelling and mechanical properties as well as studying of swelling kinetics to evaluate the possibility of hydrogels application as promising water reservoir materials.

Methods
Organic/inorganic hydrogels with double network (DN) structure based on PAANa and PAPTMS were prepared by one-pot simultaneous cross-linking processing, which includes a combination of free radical polymerization of AANa, hydrolysis of silica precursors and catalytically-induced condensation of the resulting hydroxyl groups of APTMS to form a network structure.
The cross-linking of PAANa was verified by the absence of C=C double bond as well as DN structure formation was performed by FTIR. The swelling behaviour was evaluated in distilled water at room temperature.

Results
The DN structure formation was proved by FTIR. It was found that the incorporation of 10 wt.% PAPTMS enhanced the water absorbency by 316 %. The swelling behavior of the hydrogel composites is non-Fickian, the swelling process fits the Schott's model [1] at low PAPTMS concentration.

Conclusions
The synthesized hydrogels show enhanced swelling capacity and can be considered as promising water reservoirs. The incorporation of PAPTMS into the polymeric matrix confirmed by FTIR spectroscopy and its amount greatly influences on swelling/deswelling kinetics and swelling ratio.

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TRANSPARENT POLYURETHANE MATERIALS WITH EFFECTIVE DAMPING ABILITY AND ULTRAVIOLET PROTECTION

Natalia Babkina, Lyudmyla Kosyanchuk, Liubov Vorontsova, . Oksana Antonenko, . Taisa Ignatova

Institute of Macromolecular Chemistry of the NAS of Ukraine, Kyiv

Keywords
Polyurethane, damping ability, ultraviolet protection, transparency

Actuality and aim
The development of modern technologies requires the creation of new polymeric materials with different functional properties. The aim of these studies is to obtain PU materials that would combine high damping ability and effective UV protection.

Methods
Optical microscopy, UV-Visible spectroscopy, dynamic mechanical analysis (DMA)

Results
PUs based on aliphatic and aromatic diisocyanate (DI), oligoesters, and oligoethers with different molecular weights were synthesized. Their damping properties and UV absorption have been studied. All PUs have effective damping ability, high (~ 90 %) transmittance in the visible range, and UV absorption. PUs based on aliphatic DI absorb UV up to 250–280 nm, but absorption of PUs based on aromatic DI shifts to the long-wavelength region – up to 300–400 nm due to the presence of aromatic rings. The highest UV absorption is observed for PU based on aromatic DI and ester which is due to the higher absorption capacity of ester groups relative to ether groups [1].

Conclusions
Transparent PU materials with high damping ability and effective protection of UV-A (320–400) nm and UV-B (280–320) nm were obtained. Therefore, the possibility of varying the components for the synthesis of PU allows for obtaining new high-performance damping polymeric materials with selective UV protection.

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Po-54

PREPARATION OF MAGNESIUM ALLOY AZ31 CORROSION PROTECTION COATINGS BY COMBINING PEO AND SPRAY PYROLYSIS METHODS

Reinis Drunka [1], Paula Iesalniece [2], Ints Steins [2], Liga Grase [3], Toms Valdemars Eiduks [3]

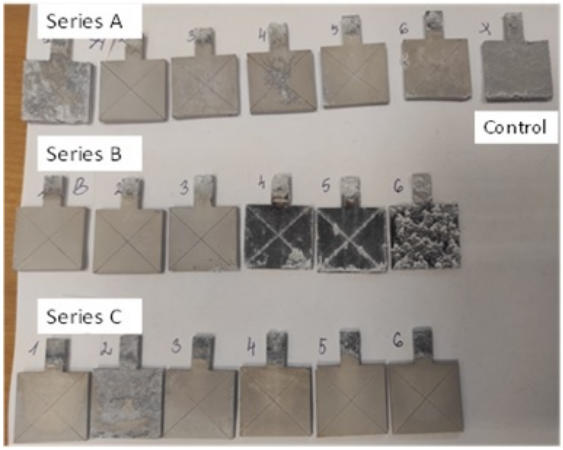
[1.] Riga Technical University, Faculty of chemistry, Institute of materials and surface engineering, Latvia; Company SMW group, [2.] Riga Technical University, Faculty of chemistry, Institute of materials and surface engineering, Latvia; Company SMW group , [3.] Riga Technical University, Faculty of chemistry, Latvia, Institute of materials and surface engineering

Keywords
PEO, AZ31, Magnesium, Corrosion, Spray pyrolysis

Actuality and aim
Today's aerospace and automotive industries have sought to use ever-lighter metals to reduce fuel consumption. Mg and its alloys are also attracting the attention of scientists, as these materials have a density of up to 30% lower than aluminum, but its widespread use is hindered by the high activity of the metal and its poor corrosion resistance. Known corrosion methods do not provide sufficient corrosion resistance, so new ways to improve a lready known methods are being sought.

Methods
The plasma electrolytic oxidation (PEO) method is similar to anodizing, but occurs at much higher voltages. During the process, a micro-spark discharge takes place on the surface, which allows to obtain a dense oxide layer on Mg alloys. If a bipolar current source with pulsed power supply is used during the PEO process, it isposs ible to homogeneously supplement the protective layer with various modifiers at the same time. However, the PEO method has drawbacks - the main one - the resulting coating is porous. To compensate for this, the possibi lities of filling additional pores by spray pyrolysis (SP) were considered in this study. The corrosion resistance of the obtained samples was evaluated by immersion method. Surface morphology, phase and chemical compos ition were assessed.

Results
The resulting coatings are able to withstand more than 168h in 3% NaCl solution without significant corrosion defects.



Corrosion test results. Surface modified with SP method by adding: a) ZnO; b) ZnO+P; C) P .

Conclusions
Combining PEO and SP methods, as well as adding small amounts of Si, P and Zr elements to the raw material solutions, significantly improves the corrosion resistance of the resulting coating.

Acknowledgements
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PHYSICAL AND CHEMICAL WATER-SORPTION PROCESSES IN THE $MGAL_2O_4$ CERAMICS

Halyna Klym [1], Ivan Karbovnyk [2], Analoti I. Popov [3]

[1.] Lviv Polytechnic National University, Ukraine, [2.] Ivan Franko National University of Lviv, Ukraine, [3.] Institute of Solid State Physics, University of Latvia

Keywords
ceramics, positron, positronium, nanopores

Actuality and aim
Dielectric humidity-sensitivity ceramics such as $MgAl_2O_4$ spinel is determined by processes of physical and chemical sorption of water occurring in their internal external defects and nanopores. In this work a water-sorption processes in the $MgAl_2O_4$ ceramics were studied by positron annihilation lifetime (PAL) spectroscopy.

Methods
The study of positron trapping defects caused by water molecules in adsorption/desorption cycles in $MgAl_2O_4$ ceramics sintered at 1400 °C for 2 hours was carried out in a specially designed humidity chamber at ambient temperature of 20 °C and relative humidity RH = 5% - 40% - 60% -98% and RH = 40% - 60% - 80% - 98% - 80% -60% - 40%.

Results
In the case of experiment in adsorption-desorption cycles the lifetime of the third component was fixed in the level of 1.9 ns. Sorption influences are reflected in intensities I1 and I2.
It was shown [1] that positron annihilation processes in $MgAl_2O_4$ ceramics are adequately described by multichannel model. The first component of the PAL spectra reflects the basic microstructural features of spinel ceramics, the second one corresponds to defects localized near grain boundaries, and the third one describes the “pick-off” annihilation of o-Ps in nanopores.

Conclusions
The intensity of the first component decreases with adsorption of water by nanopores of ceramics, but increases at desorption. The intensity of I2 increases with relative humidity RH change from 40% to 98% and decreases when RH changes from 98% to 40%.
The intensity of the third component does not change and remains at the level of 1%. With such adsorption-desorption cycles in $MgAl_2O_4$ ceramics, this positron annihilation channel is insensitive to physically adsorbed water.

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MODELLING OF THE SCATTERING SPECTRUM OF METAL NANOPARTICLES ON POROUS ANODIZED ALUMINIUM OXIDE OF VARIOUS THICKNESS

Aušrinė Jurkevičiūtė, Juris Prikulis

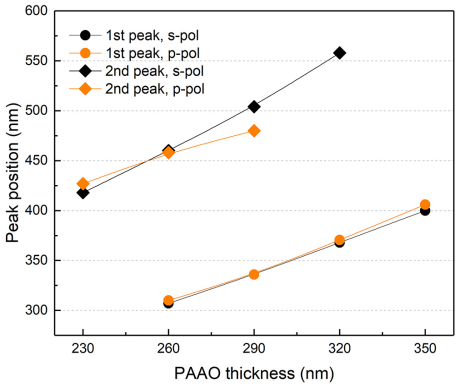
University of Latvia

Keywords
FDTD, PAAO, light scattering, modelling, gold nanoparticles

Actuality and aim
Porous anodized aluminium oxide (PAAO) is a versatile material with the potential to be applied in optical sensors, especially when combined with metal nanoparticles [1]. The sensitivity of the sensor is related to the features of the light spectrum after interaction with the sample. Therefore, the sensitivity of the sensor depends on the materials and geometry of the sensor elements.

Methods
In this work, we employ finite-difference time-domain (FDTD) modelling of light scattering from PAAO covered with gold nanoparticles (Au NPs). Geometric parameters are taken from [1], pores are considered to have a perfect 6-fold symmetry, and there is an Au NP in each pore. We change the thickness of the PAAO and record the spectrum of scattered light.

Results
It is possible to distinguish two clear peaks in the scattered spectrum for each PAAO thickness. The positions of the peaks in scattered light spectra depend linearly on the thickness of PAAO in the lower visible and ultraviolet ranges (see figure). From around 550 nm wavelength and towards the infrared region, the peaks become very broad, and the intensity of scattered light is increasing.



The relation between scattering peaks positions and the PAAO thickness for s- and p-polarized light

Conclusions
The chosen geometry for optical sensors based on porous anodized aluminium oxide and gold nanoparticles depends on the light source to be used in the setup. In the wavelength range of the light source, there should be a clear, sharp peak. From our modelling it was determined that if the light source is in the visible range, a suitable PAAO thickness in around 290 nm. Lower thickness might result in out-of-range peak values of the light source. A larger thickness results in too broad peaks.

Acknowledgements
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[1] doi:10.3390/nano9040531

COMPARISON OF DIFFERENT COATINGS TECHNIQUES FOR ZINC OXIDE NANOPARTICLES FOR ROOM-TEMPERATURE UV SENSORS

Mindaugas Ilickas [1], Brigita Abakevičienė [1], Rasa Mardosaitė [2], Simas Račkauskas [1]

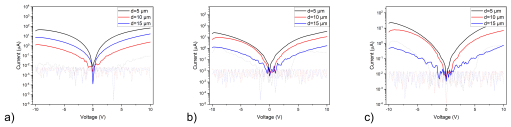
[1.] Department of Physics, Kaunas University of Technology, Studentų St. 50, LT-51368 Kaunas, Lithuania; Institute of Materials Science of Kaunas University of Technology, K. Baršausko St. 59, LT-51423, Kaunas, Lithuania, [2.] Institute of Materials Science of Kaunas University of Technology, K. Baršausko St. 59, LT-51423, Kaunas, Lithuania

Keywords
ZnO nanowire, UV sensor, spray-coating, drop-casting

Actuality and aim
ZnO nanowire UV sensors have very high ON/OFF ratios between IUV and IDark currents due to their large surface area [1] and 1D structure [2]. The aim of this work is to optimize ZnO nanowire deposition methods to obtain UV sensors with a quick response to low UV light at room temperature, which can be potentially used in flexible electronics.

Methods
An X-ray diffractometer was used to investigate the structural characterisation of ZnO nanowires. A scanning electron microscope (SEM) was used to evaluate morphological properties. A Keithley 6487 picoammeter was used to measure the current-voltage characteristics.

Results
The highest ON/OFF ratio, using UV light intensity of 0.31 mW/cm^2, has been obtained by spray-coating technique with an inter-electrode gap of 5 μm – 2182.63, and the lowest ON/OFF has been obtained using a drop-casting technique (big drops) at an inter-electrode gap of 15 μm – 14.13.



I-V curves of ZnO coated by various methods: a)spray-coating b)small drop-casting c)big drop-casting

Conclusions
The best ON/OFF ratio for UV sensors was obtained for the spray-coating technique (105.7 to 2182.8). The drop-casting technique results in ON/OFF from 35.52 to 175.02 and 11.13 to 995.95 for small drops and big drops, respectively. The varied number of contacts between inter-electrode gaps can be explained by the drop evaporation front produced conditions.

Acknowledgements
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SYNTHESIS OF GRAPHENE ON SI(100) USING DIRECT MW-PECVD AND PROTECTIVE ENCLOSURES

Šarūnas Jankauskas, Rimantas Gudaitis, Algirdas Lazauskas, Šarūnas Meškinis

Institute of Materials Science of Kaunas University of Technology, K. Baršausko st. 59, LT-51423, Kaunas, Lithuania

Keywords
graphene, direct synthesis, MW-PECVD, shielding

Actuality and aim
Graphene is known to possess many properties that are superior to other materials used in optoelectronics. Currently, graphene's potential is hindered by its small scale growth. To overcome this, microwave plasma-enhanced chemical vapor deposition (MW-PECVD) is used to produce graphene on various dielectric and semiconductor substrates [1]. By combining protective plasma shielding enclosures, this method could ensure a large-scale graphene synthesis.

Methods
Graphene was grown on the Si(100) substrates by using MW-PECVD system (IPLAS Innovative Plasma Systems GmbH). 3 circular protective steel enclosures with different hole diameters and arrangements on top (3.5 mm, 2 mm and 3.5 mm with no holes at the top respectively) were used in its synthesis, while 4th enclosure had a simple open ended rectangular configuration. Samples were analyzed using Raman spectroscopy (Renishaw inVia, 532 nm) by evaluating I2D/IG and ID/IG ratios.

Results
Based on Raman spectra findings, CH_4/H_2 ratio as low as 0.11 produces no graphene, while 0.33 gives a clear graphene fingerprint. Further increase of CH_4/H_2 ratio increases the number of layers as evident from the decrease of I2D/IG. No enclosure design effects on produced graphene were found.

Conclusions
As it appears, graphene can be successfully grown using MW-PECVD method with a simple protective enclosure design as a means to suppress direct plasma effects on the sample. We also show that most detrimental parameter in such synthesis is the CH4/H2 flow ratio.

Acknowledgements
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DESIGNING OF EXPERIMENTAL SETUP FOR IMPACT INDUCED MECHANOLUMINESCENCE MEASUREMENTS

Syed Shabhi Haider [1], Justyna Barzowska [2], Piotr Sybilski [1], Andrzej Suchocki [1]

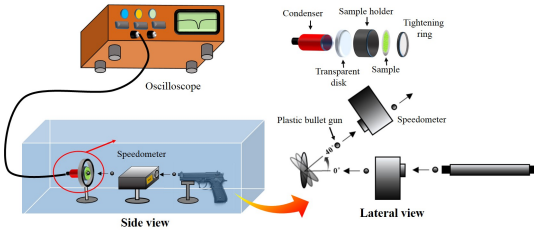
[1.] Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, Warsaw 02-668, Poland., [2.] Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, ul. Wita Stwosza 57, 80-952 Gdansk, Poland

Keywords
Impact induced mechanoluminescence; impact sensor, mechanoluminescent

Actuality and aim
An alternative and integrative approach has been adopted to construct an unique low-cost laboratory equipment for measuring the mechanical impact-induced mechanoluminescence (I-ML) properties of materials.

Methods
This apparatus consists of an electric gun, speedometers, targeted cylinder, condenser followed by optical fiber, photomultiplier, and digital oscilloscope. To measure the I-ML, a spherical projectile with a known mass is fired at the target plate have ML sample, results sudden emission of photons from the material, detected by the photomultiplier. An electrical signal generated by the photomultiplier is recorded. The intensity and duration of the resulting electrical signal are directly related to the number of emitted photons after the absorption of energy by the ML material. Furthermore, we systematized it more versatile by using a rotatable sample holder which easily rotates at different incident angles for variable deposited energy transfer.

Results
The extracted I-ML results for luminescence powders $Sr_{0.95}Ca_{0.05}(SO_4)$:Eu and $SrAl_2O_4$:Eu,Dy validates the satisfactory performance of the constructed I-ML setup. The design and handling of the proposed setup are simple and highly beneficial for comprehensive experimental analysis of the I-ML characteristics.



The schematic illustration of self-designed I-ML measurement setup.

Conclusions
The setup is capable of investigating the various impact kinetic energy-dependent luminescence signal in the range of 200 mJ to 269 mJ using 0.28 g sphere projectiles with high sensitivity. Such an integrative approach to designing a low-cost (~100 €), simple and user-friendly setup helps in exploring the I-ML behavior of ML materials, useful for the advancement of impact detection and stress transformation.

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PREPARATION AND TRIBOLOGICAL PROPERTIES OF MULTILAYER TUNGSTEN OXIDE NANO SMART COATINGS

Dr Vera Skvortsova [1], Martins Zubkins [1], Viktors Vibornijs [1], Jelena Arhipova [1], Juris Purans [1], Armands Leitans [2], Janis Lungevics [2]

[1.] Institute of Solid State Physics, University of Latvia , [2.] Institute of Mechanics and Mechanical Engineering, Riga Technical University, Latvia

Keywords
Tungsten oxide; Magnetron sputtering; Tribology

Actuality and aim
The COVID-19 pandemic has intensified the world's attention toward the spread of contamination facilitated by high touch surfaces. Such coatings should provide a combination of good mechanical and tribological characteristics. A newly emerging field of application involving tungsten oxide based compounds is as antimicrobial agents in healthcare industry [1]. In this work deposited by magnetron sputtering multilayer tungsten oxide thin films tribological properties are studying.

Methods
Thin film coatings of WO_{3-x}/Cu/WO_{3-x} and WO_{3-x}:Cu , WO_{3-x} and Cu were deposited using direct current magnetron sputtering (DCMS) techniques from W (purity 99.95 %) and Cu (purity 99.99 %) targets.
Tribological properties of the coatings were measured with a tribometer according to ASTM G99 standard. After coefficient of friction measurement, determine coating wear rate, with a surface profilometer. The adhesion of thin-film coating was evaluated with scratch test, also by Rockwell C indentation test according to DIN 4856: 2018-02.

Results
The coatings were applied to soda-lime glass, PET and hardened steel. All the deposited WO_{3-x}/Cu/WO_{3-x}, WO_{3-x}:Cu coatings are X-ray amorphous regardless of sputtering regime or deposition parameters. Coefficient of friction values range from 0.21 to 0.53. In all samples wear has been detected. Coating types reveal few spalling failures around the indent edge and are categorized into adhesion class HF1-5.

Conclusions
It is shown that for the synthesis of effective antibacterial coatings, it is necessary to take into account the influence of the main sputtering parameters (type and pressure of the working gas, substrate displacement potential, target, etc.) as well as the tribological properties.

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THE USE OF TUNGSTATE NANOPARTICLES IN HYBRID X-RAY DETECTORS

Inga Pudza, Kaspars Pudzs, Georgijs Bakradze, Janis Cipa, Andrejs Tokmakovs, Alexei Kuzmin

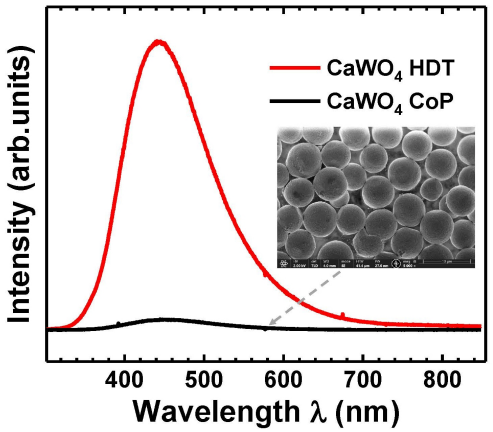
Institute of Solid State Physics, University of Latvia

Keywords
Tungstates, nanoparticles, XRD, SEM, X-ray absorption spectroscopy

Actuality and aim
Tungstates of divalent metals form a large class of materials with various applications including but not limited to scintillators, photocatalysis, supercapacitors and sensors. The high value of the atomic number of tungsten (Z=74) and the possibility to vary the atomic number of the second cation in a wide range (Z=12 for Mg, Z=56 for Ba) make tungstates attractive for the development of novel hybrid organic-inorganic X-ray detectors.

Methods
In this study, scheelite (A=Ca, Sr) and wolframite-type (A=Zn, Cd) tungstates with different crystallinity were prepared using co-precipitation (CoP) and hydrothermal (HDT) synthesis. Nano- and polycrystalline powders were characterized by XRD, scanning electron microscopy (SEM), X-ray absorption spectroscopy (XAS), Raman spectroscopy and X-ray excited optical luminescence (XEOL).

Results
Different synthesis parameters affect the size and morphology of nanoparticles (NPs). CoP at room temperature results in agglomerated NPs with an average size of 15-30 nm, but using citric acid as a capping agent the average size of NPs was smaller than 5 nm. However, XEOL is suppressed in NPs with low crystallinity because of high lattice defect concentration (see figure). In XAS spectra, size-induced local structure relaxations are observed which are more pronounced in NPs of wolframite-type. The HDT synthesis results in highly crystalline NPs with improved XEOL.



XEOL of two $CaWO_4$ samples.
A SEM micrograph of CaWO4 microspheres isshown in the inset.

Conclusions
We show that the best sensitivity to X-rays is determined by a subtle interplay between particle size and their crystallinity.

Acknowledgements
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LUMINESCENCE OF DOPED ALN MATERIALS

Rihards Ruska, Baiba Bērziņa, Jānis Čipa , Laima Trinklere

Institute of Solid State Physics, University of Latvia

Keywords
Luminescence, aluminium nitride, manganese, europium, chromium

Actuality and aim
Phosphors that emit red light (RL) are frequently utilized in biomedical research [1], entertainment, and safety indicators. Aluminum nitride (AlN) based RL emitters are intriguing prospects for new such materials because of their low toxicity and wide bandgap. Even though the luminescence of doped AlNs have been studied at room temperatures, other spectral features and mechanisms underlying them are largely unknown.

Methods
Luminescence processes of europium, manganese, and chromium-doped AlN materials (AlN:Eu, AlN:Mn, and AlN:Cr) were investigated using photoluminescence (PL) and its excitation (PLE) spectra as well as kinetics. Studies were performed at different temperatures (10 – 300 K) and environments (vacuum and air).

Results
We found that AlN:Eu PL peaked at 530 nm, AlN:Mn – at 600 nm, but AlN:Cr – at 690 nm. These luminescent bands in AlN could be excited both via intra-center and recombination mechanisms. Moreover, presence of similar recombination excitation bands and persistent luminescence were detected in both AlN:Eu and AlN:Mn samples. PLE-PL kinetics were used to confirm assumptions about process mechanisms.

Conclusions
Our findings will be further used to develop novel bicycle safety equipment based on doped AlN.

Acknowledgements
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DIFFERENT STRATEGIES FOR GAN-MOS_2 AND GAN-WS_2 CORE–SHELL NANOWIRE GROWTH

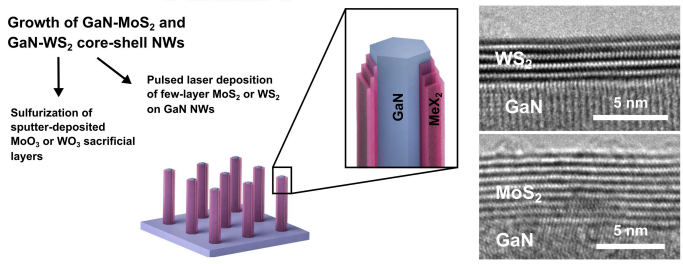
Boris Polyakov

Institute of Solid State Physics, University of Latvia

Keywords
Nanowire, GaN, MoS_2, WS_2, Core–shell Heterostructure

Actuality and aim

One-dimensional (1D) nanostructures – nanowires (NWs) – exhibit attractive properties for integration in different types of functional devices. Their properties can be enhanced even further or tuned for a specific application by combining different promising materials, such as layered van der Waals materials and conventional semiconductors, into 1D-1D core–shell heterostructures. In this work, we demonstrated growth of GaN-MoS_2 and GaN-WS_2 core–shell NWs via two different methods: (1) two-step process of sputter-deposition of a sacrificial transition metal oxide coating on GaN NWs followed by sulfurization; (2) pulsed laser deposition of few-layer MoS_2 or WS_2 on GaN NWs from the respective material targets. As-prepared nanostructures were characterized via scanning and transmission electron microscopies, X-ray diffraction, micro-Raman spectroscopy and X-ray photoelectron spectroscopy. High crystalline quality core–shell NW heterostructures with few-layer MoS_2 and WS_2 shells can be prepared via both routes. The experimental results were supported by theoretical electronic structure calculations, which demonstrated the potential of the synthesised core–shell NW heterostructures as photocatalysts for efficient hydrogen production from water.



Acknowledgements

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E. Butanovs, K.Kadiwala, A.Gopejenko, D.Bocharov , S. Piskunov, B.Polyakov, Applied Surface Science 590 (2022) 153106

THIN FILMS OF WSE_2 SYNTHESIZED VIA SELENIZATION OF WOX AND W PRECURSOR MATERIALS FOR COMPARISON

Kevon Kadiwala, Edgars Butanovs, Andrejs Ogurcovs, Martins Zubkins, Boris Polyakovs

[1.] Institute of Solid State Physics, University of Latvia, Kengaraga street 8, Riga, Latvia, LV-1063

Keywords
Tungstendiselenide,Transitionalmetaldichalcogenides,photolithography

Actuality and aim
To compare the synthesized WSe_2 crystalline films from each precursor material and understand how they affect the different properties of the WSe_2 films.

Methods
CVT method is one of the most efficient, widely used and upscalable 2D materials synthesis techniques available[1], therefore, here WSe_2 films are also synthesized using that method keeping in mind possible upscaling in future.

Results
WSe2 films synthesized from the WO3 precursor material, showcased more crystals growing out-of-plane compared to the films synthesized from W metal precursor. SEM images and AFM images confirms these findings. XRD and Raman measurements confirm the material of the films to be WSe_2. Photoelectric devices made from WO_3 precursor seem to perform better when compared to devices made from 'W' precursor films. WSe_2 crystals are prone to vacancy defects and lack of oxygen atoms to passivate the selenium vacancies in films made from 'W' might be the reason for degraded photoelectric properties.

Conclusions
- SEM and AFM images showed the films grown from metal W precursor had significantly lower surface roughness than the films grown from WO_3 precursor.
- Films made from W precursor, crystal sizes were noticeably smaller (~0.4 μm) in comparison to the films made from WO_3 (~0.8 μm) which had crystal growth in random orientation.
- Photoelectric measurements revealed that despite having the out-of-plane crystal growth on the film from the WO_3 precursor, films showed higher photocurrent and stability which was not the case with planar crystals grown from the metal W precursor.

Acknowledgements
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LOW FREQUENCY NOISE CHARACTERISTICS OF COMPOSITES WITH MWCNT AND NI@C NANOPARTICLES

Marina Tretjak, Deividas Žiūraitis, Martynas Juozaitis, Sandra Pralgauskaitė, Darya Meisak, Jan Macutkevič, Jūras Banys, Jonas Matukas

Institute of Applied Electrodynamics and Telecommunications, Lithuania

Keywords
fluctuation, noise, MWCNT, Ni@C, composite

Actuality and aim
The composites filled with multi-walled carbon nanotubes (MWCNTs) and carbon-coated Ni nanoparticles (Ni@C) provide a wide range of features what enables more optimal solutions for modern technologies and applications of such materials [1,2]. Low frequency noise characteristics of MWCNT and Ni@C composites were investigated with the aim to clear up physical processes that determine possibilities and limitations of these composites usage in electronics.

Methods
Low frequency noise (voltage fluctuations) and resistivity characteristics were measured under constant current mode in the frequency range from 10 Hz to 20 kHz at temperatures from 75 K to 375 K. The noise measurements were performed in a special laboratory room – Faraday cage.

Results
The low frequency noise and resistivity measurement results show that addition of the MWCNTs to the Ni@C and dielectric composite increases temperature at which increase of the material conductivity starts. It was observed that for particular samples with a higher concentration of conductive Ni@C particles, electrical resistance was larger comparing with composites with a lower filler concentration. This can be due to the more homogeneous distribution of the conductive particles what prevents from formation of good percolation network. Also, in the former, noise increase was observed when temperature cycles were repeated.

Conclusions
Addition of MWCNTs in the composites with Ni@C filler causes larger material resistivity to the thermal effects. The more homogeneous distribution of the Ni@C particles in the dielectric matrix (when material is above the percolation threshold) is related with the larger noise observed during the repeating temperature cycles.

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COMPARISON OF METHODS FOR INTEGRATION OF BI2SE3 NANOWIRES IN NEM SWITCHES

Elza Dzene, Līga Jasulaņeca, Raitis Sondors, Edijs Kauranens, Jana Andžāne, Donāts Erts

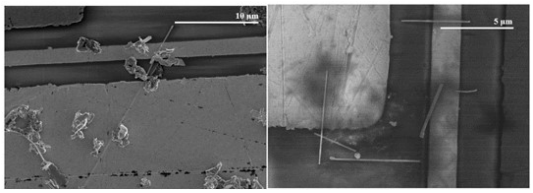
Institute of Chemical Physics of the University of Latvia

Keywords
Bi_2Se_3, DEP, nanoelectromechanical switch

Actuality and aim
Nanoelectromechanical or NEM switches are nanoscale energy-efficient devices that allow the transmission of electrical signals through mechanical and electrical interactions. Whenfabricated using Bi_2Se_3 nanowires as the active elements, they are able to operate at extremely low temperatures.

Methods
In this work, two different nanowire transfer methods are used to create NEM switches - mechanical pressing and dielectrophoresis. They are compared with each other and combined to obtain as many clean devices as possible without the presence of other nanostructures. The operation of the as-fabricated NEM switches is characterized at temperatures as low as 5 K.

Results
Experiments have shown that mechanical nanowire transfer can break the longest nanowires, but no excessive number of unwanted nanoparticles is observed. On the other hand, when nanowires are transferred using dielectrophoresis, they do not break, which provides better device contacts, but the presence of unwanted nanostructures is inevitable.



Schematics for mechanical transfer of nanowires and their transfer using dielectrophoresis

Conclusions
By combining the two nanowire transfer methods into one, it is possible to obtain clean devices without the presence of unwanted nanoparticles. NEM switches show repeatable switching at cryogenic temperatures as low as 5 K.Further efforts need to be devoted to increasing the yield of aligned nanowires using dielectrophoresis.

Acknowledgements
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FEMTOSECOND LASER ABLATION AT 1030 NM, SECOND HARMONIC AND THIRD HARMONIC FOR NITROCELLUECE MEMBRANE

Gazy Khatmi [1], Mohamed Ahmed Baba [2], Martynas Simanavičius [3], Laimis Silimavičius [3], Tomas Tamulevičius [4]

[1.] Kaunas University of Technology Faculty of Mathematics and Natural Science I Physics, Lithuania, [2.] Institute of Materials Science, Kaunas University of Technology, Lithuania, [3.] UAB Sanpharm, Lithuania, [4.] Department of Physics, Kaunas University of Technology, Lithuania 2 Institute of Materials Science, Kaunas University of Technology,UAB Nanoversa, Lithuania

Keywords
Nitrocelluece membrane, Ablation, Femtosecond laser

Actuality and aim
Nitrocellulose membranes are widely used in lateral-flow immunoassays (LFA) for different purpose diagnostic tests where the fluid sample added to the membrane flows through the LFA by capillary forces, interacting with detection antibody-labeled gold nanoparticles [1]. Ultrashort lasers enable cold ablation of porous materials and were already applied for imposing surface structures and wettability handling aiming for bio sensing applications [3-5]. In this work, we determined the ablation threshold of tow type of membrane by different femtosecond wavelength. In addition, we are demonstrating a technique for the fabrication of hydrophilic channels in nitrocellulose membranes using a femtosecond laser micromachining system

Methods
Nitrocellulose membranes from were investigated:
Carl ROTH Gmbh&CO: pore size 0.45 µm
Rot@NC: pore size 0.2 µm.
Membranes were µ-machined with fs-laser:

Yb:KGW (Pharos, Light Conversion), 280 fs, 40 kHz,
FH λ=1030 nm, 2H λ=515 nm, 3H λ=343 nm.
FemtoLab workstation (Altechna R&D): XYZ (Aerotech), light focused with microscope objective (Mitutoyo) or aspherical lens.
SEM Quanta 200 FEG (FEI) used for surface microanalysis

Results
Two types of nitrocellulose membranes of different porosity were structured with femtosecond laser using 1030 nm, 515 nm, and 343 nm wavelength and ablation thresholds were determined: 0.25 µJ, 0.25 µJ, and 0.75 µJ respectively

Conclusions
Two types of nitrocellulose membranes of different porosity were structured with femtosecond laser using 1030 nm, 515 nm, and 343 nm wavelength and ablation thresholds were determined: 0.25 µJ, 0.25 µJ, and 0.75 µJ respectively

Acknowledgements
The work was supported by the Agency for Science, Innovation and Technology, Grant No. Biotech-02-014.

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GRAPHENE GAS SENSORS GRAFTED WITH TiO_2 NANOLAYERS: TEMPERATURE DEPENDENCE OF NO_2 RESPONSE

Paniz Vafaei, Raivo Jaaniso, Margus Kodu

Institute of Physics, University of Tartu, W. Ostwald Street 1, EE50411 Tartu, Estonia

Keywords
Graphene - TiO_2 - Pulsed laser deposition -Gas sensor - NO_2- Adsorption-Modelling

Actuality and aim

NO_2 is one of the air pollutants that must be monitored in the environment at sub-ppm levels. Recently, several graphene-based gas sensors with improved sensitivity have been implemented [1,2]. Here, we demonstrate the functionalization of single-layer graphene (SLG) by pulsed laser deposition (PLD) to prove that graphene is compatible with TiO_2 thin film, and model the response and recovery kinetics of NO_2 sensing to evaluate the activation energies of sorption processes.

Methods

SLG was grown on Cu foil via the CVD and transferred using PMMA as a transfer film to the top of Si/SiO_2 substrates with Ti/Au electrodes, then 0.5 nm of TiO_2 was grown on graphene by PLD (Fig1b). Measurements were carried out in the flow-through chamber at 50-250 °C in exposure to 40-300 ppb of NO_2 while N_2 and O_2 were used as carrier gases.

Results

The gas responses (Fig. 1a) were fitted to (bi)exponential functions and rate constants were determined for both adsorption and desorption processes of NO_2. The Arrhenius plots of rate constants (Fig. 1b) yielded the respective activation energies and proportions of different binding sites.

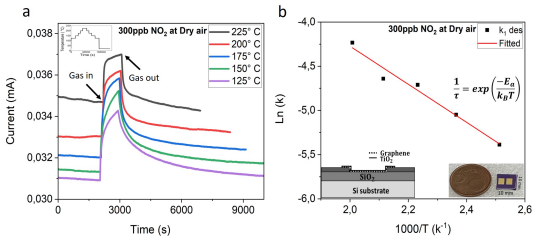


Fig.1. a. Dynamic responses of sensor; b. Arrhenius plot based on the rate constants got by fitting.

Conclusions

Activation energy of desorption was 0.18 eV, whereas it was close to zero (certainly < 0.1 eV) for adsorption in dry air or N_2 as a carrier gas. DFT calculations of these parameters are in progress.

Acknowledgements

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TIME RESOLVED LUMINESCENCE STUDY OF PR^{3+} DOPED LUPO4 NANOCRYSTALS SYNTHESIZED IN AQUA-ORGANIC SOLVENT.

Sanu Bifal Maji, Marco Kirm, Alexander Vanetsev, Eduard Feldbach, Vitali Nagirnyi, Juhan Saaring

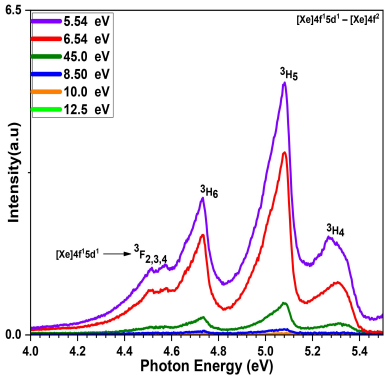
University of Tartu, Estonia

Keywords
Synchrotron Radiation, interconfiguration Pr^{3+} $4f^15d^1 \rightarrow 4f^2$ transitions , UV-C

Actuality and aim
Radiotherapy is one of the techniques used for treating a wide variety of cancers. In this treatment, high-energy X-ray radiation damages tumor cells. DNA of cells shows a characteristic absorption in the UV range from 230 nm to 280 nm (λ_{max} -260 nm) [1]. Introducing the nanocrystals, which emit UVC radiation in the patient body, will cause direct and indirect damage to DNA, increasing the efficiency of radiotherapy. Our research focuses on developing highly efficient phosphate-based nanocrystals that emit UV-C photons upon X-ray exposure.

Methods
$LuPO_4$:Pr(1%) nanocrystals were synthesized using the solvothermal synthesis method at 200°C for 3 hours in different mixtures of aqua-organic solvents using $Lu(NO_3)_3$, $Pr(NO_3)_3$, and $(NH_4)_2HPO_4$ Precursor materials.

Results
SEM and XRD studies show the tetragonal crystal structure with crystallite sizes 8, 10, and 13 nm. Cathodoluminescence spectroscopy and synchrotron radiation studies revealed the UV-C emissions due to interconfiguration Pr^{3+} $4f^15d^1 \rightarrow 4f^2$ transitions in $LuPO_4$:Pr^{3+}(1%) nanocrystals. Observed shortening of decays Pr^{3+} $4f^15d^1 \rightarrow 4f^2$ transitions is assigned to quenching processes in nano-size powder.



Pr^{3+} $4f^1$ $5d^1 \rightarrow 4f^2$ emissions in LuPO4:Pr nanocrystals excited by photons at different energies

Conclusions
UV-C emissions from $LuPO_4$:Pr^{3+} nanocrystals were successfully revealed under inter-configuration $4f^2 \rightarrow 4f^1$ $5d^1$ excitation of Pr^{3+} ions and e-beam excitation of LuPO4 host material

Acknowledgements
University of Tartu
FinEstBeAMS Max(IV) Laboratory, Sweden.

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STUDY OF THE RHODAMINE 6G PHOTODEGRADATION EFFICIENCY WITH DIFFERENT POLYDOPAMINE SHELL THICKNESS AU/PDA NANOPLATFORMS

Daniel Aguilar Ferrer [1], Emerson Coy [2], Mikhael Bechelany [3], Igor Iatsunskyi [2], Sergio Moya [4]

[1.] NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614, Poznan, Poland and Institut Europeen des Membranes, IEM, UMR 5635, Univ Montpellier, ENSCM, CNRS, 34730 Montpellier, France, [2.] NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614, Poznan, Poland, [3.] Institut Europeen des Membranes, IEM, UMR 5635, Univ Montpellier, ENSCM, CNRS, 34730 Montpellier, France, [4.] Centre for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), Paseo Miramon 182 C, 20014 Donostia-San Sebastian, Spain

Keywords
Polydopamine, gold nanorods, photodegradation, Rhodamine 6G, photocatalysis

Actuality and aim
By combining gold nanoparticles with other materials such as polydopamine (PDA) their performance in the catalytic field can be improved [1,2]. Here, The aim is to synthesize different PDA shell thickness Au rods nanoplatforms (AuNRs/PDA) and study their interface towards Rhodamine 6G (Rh6G) photodegradation.

Methods
The synthesis process consisted in a seed-mediated growth [3] followed by the formation of the final PDA cover. Obtained materials were examined with Transmission Electron Microscopy (TEM) and Localised Surface Plasmon Resonance (LSPR) with Ultraviolet-Visible (Uv-Vis) spectroscopy. The concentration of gold was unveiled with Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Photocatalysis was carried out with a xenon lamp and examined with Uv-Vis spectroscopy.

Results
Several hybrid nanoplatforms (AuNRs/PDA) were synthesized showing different PDA shell average thicknesses from ≈ 4 nm to ≈ 30 nm with LSPR values between 920 nm and 800 nm. Different PDA thickness nanoplatforms were tested in Rh6G photodegradation. The highest performance was observed for the sample with an average shell thickness of: 30.45 ± 4.9 nm, depleting almost 35% of Rh6G initial concentration in 1h for a relatively small concentration ([AuNRs] = 9815.60 µg/L).

Conclusions
This work shows that different shell thickness AuNRs/PDA can be synthesized and that they could be used as a model for enhanced organic dye photocatalysis.

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FAST MICROWAVE ASSISTED SOLVOTHERMAL SYNTHESIS OF MAGNETITE NANOSPHERES

Lina Mikoliunaite, Greta Zambzickaite, Martynas Talaikis, Gediminas Niaura

Department of Organic Chemistry, Center for Physical Sciences and Technology, Lithuania

Keywords
Magnetite, Fe_3O_4, Microwave assisted solvothermal synthesis

Actuality and aim
Synthesis of magnetic nanoparticles triggers the interest of many scientists due to their many interesting properties and wide range of application in biomedicine [1]: starting from MRI contrast agents, drug delivery systems, magnetic separators or hyperthermia agents followed by environmental [2], catalysis [3] or biosensing [4] fields.

Methods
In this work organic magnetite synthesis using microwave assisted solvothermal synthesis is investigated. Fe_3O_4 nanospheres were prepared using $FeCl_3$ as an iron source, ethylene glycol as solvent and reductor, and sodium acetate as precipitating and nucleating agent. Influence of the presence of PEG as additional reductor and heat absorbent was also evaluated.

Results
Here the synthesis time was reduced to 1 min by increasing reaction temperature using microwave reactor under pressure or add PEG at lower temperatures. The obtained magnetite spheres are 200–300 nm in size and they are composed of 10–30 nm size crystallites. After investigation, it was determined, that adding PEG results in spheres with mixed magnetite and maghemite composition and synthesis time increase the size of crystallites.

Conclusions
This work provides a comprehensive analysis of the magnetic nanoparticles synthesized using microwave assisted solvothermal method. We hope, that this research will be beneficial for the further synthesis, development and applications of magnetite nanoparticles.

Acknowledgements
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NANOSTRUCTURED BI2SE3 THIN FILMS AS A PERSPECTIVE ANODE FOR AQUEOUS RECHARGEABLE LITHIUM-ION BATTERIES

Vitalijs Lazarenko [1], Yelyzaveta Rublova [2], Raimonds Meija [2], Jana Andzane [2], Vanda Voikiva [2], Artis Kons [3], Arturs Viksna [4], Donats Erts [5]

[1.] Nano RAY-T, Instituta street 36-17, Ulbroka, LV-2130, Riga, Latvia, University of Latvia, Faculty of Chemistry, Raina blvd. 19, LV-1586, Riga, Latvia, [2.] Institute of Chemical Physics, University of Latvia, Raina blvd. 19, LV-1586, Riga, Latvia, [3.] Latvia, University of Latvia, Faculty of Chemistry, Raina blvd. 19, LV-1586, Riga, Latvia, Institute of Chemical Physics, University of Latvia, Raina blvd. 19, LV-1586, Riga, [4.] University of Latvia, Faculty of Chemistry, Raina blvd. 19, LV-1586, Riga, Latvia, [5.] Institute of Chemical Physics, University of Latvia, Raina blvd. 19, LV-1586, Riga, Latvia, University of Latvia, Faculty of Chemistry, Raina blvd. 19, LV-1586, Riga, Latvia

Keywords
Bi_2Se_3 thin films, anode, aqueous rechargeable lithium-ion batteries (ARLIB).

Actuality and aim
Even though lithium-ion batteries (LIBs) have dominated the world marketplace, on the other hand, aqueous rechargeable lithium-ion batteries (ARLIBs) have attracted huge attention as the cheapest battery system. The use of lithium aqueous electrolyte reduces the risk of battery flammability and explosiveness. However, this type of battery still has serious drawbacks, such as low cycling performance and a low potential window. Bi_2Se_3 is a unique material with a layered structure that has already demonstrated great performances as an anode for LIBs and possibly this material could also be a promising candidate for ARLIBs. The aim of this research was to investigate the electrochemical performance of Bi_2Se_3 thin films with formed solid electrolyte interphase (SEI) and Bi_2O_3 layer in the lithium aqueous electrolyte.

Methods
The Bi_2Se_3 thin films were synthesized using the physical vapour deposition method. The electrochemical properties were investigated by using different analysis techniques. The analysis of surface morphology and chemical compositions scanning electron microscope and X-ray spectroscopy were used.

Results
none

Conclusions
For the first time, the results of this work show possible perspectives of Bi_2Se_3 thin films as anode for ARLIBs system and the comparison of electrochemical properties between formed SEI and Bi2O3 layer.

Acknowledgements
This research was funded by the European Regional Development Fund Project (ERDF) No. 1.1.1.1/19/A/139. V. L. acknowledges the support of “Strengthening of the capacity of doctoral studies at the University of Latvia within the framework of the new doctoral model”, identification No. 8.2.2.0/20/I/006.”. Y. R. acknowledges the support of post-doctoral ERDF project No. 1.1.1.2/VIAA/4/20/694.

INVESTIGATION OF SINGLE WALLED CARBON NANOTUBE NETWORK ANODE IN AQUEOUS $LINO_3$ ELECTROLYTE

Irina Oliseveca, Yelyzaveta Rublova, Vitalijs Lazarenko, Vanda Voikiva, Raimonds Meija, Artis Kons, Donats Erts

Institute of Chemical Physics, University of Latvia

Keywords
anode, aqueous lithium ion batteries, anode; CNT, $LiNO_3$

Actuality and aim
To provide better electron conduction pathways for anodes' active materials in non-aqueous and aqueous Li-ion batteries, carbon nanotubes (CNTs) are used [1]. While, CNTs have been widely studied both experimentally and theoretically, information about their electrochemical performance, when used as anodes in aqueous lithium electrolytes is lacking.

Methods
In this work single wall CNTs (SWCNTs) were investigated in an aqueous 5 M $LiNO_3$ electrolyte. To characterize electrochemical properties, electrochemical impedance spectroscopy at open circuit potential, cyclic voltammetry (CV) and galvanostatic charge/discharge measurements in a potential range (-0.2÷ 0.5) (vs Ag/AgCl) were performed. To identify the chemical composition and morphology, Fourier transform infrared spectroscopy, energy dispersive x-ray spectroscopy (EDX) and scanning electron microscopy (SEM) were performed.

Results
CV curves demonstrate high reversibility for Li+ intercalation/deintercalation and reveal capacitive current as the main contributor to the peak current, which can be explained by the pseudocapacitance. EIS data show, that the electrode changes the most within the first 50 cycles. SEM/EDX showed accumulation of lithium nitrate crystals on the surface of the electrode, associated with decomposition of the electrolyte.

Conclusions
The electrochemical mechanism of a SWCNT anode was determined, showing a multistep process, consisting of ion solvation, their diffusion towards the electrode surface, weak adsorption, desolvation and intercalation/deintercalation of the lithium.

Acknowledgements
This work was supported by European Regional Development Fund project No. 1.1.1.1/19/A/139 "Development of innovative binder-free anode electrodes for lithium-ion batteries".

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PROPERTIES AND APPLICATIONS OF BLENDED AND ENCAPSULATED BISMUTH SELENIDE AND CNT HYBRID STRUCTURE-BASED FLEXIBLE THERMOE

Krisjanis Buks [1], Jana Andzane [2], Loreta Brauna [2], Michael Katkov [1], Donats Erts [2]

[1.] 3D Strong Ltd., Instituta str. 36-17, LV-2130, Ulbroka, Ropazu nov., Latvia, [2.] 2Institute of Chemical Physics, University of Latvia, Raina blvd. 19, LV-1586, Riga, Latvia

Keywords
Thermoelectrics, carbon nanotubes, nanocomposites, bismuth selenide

Actuality and aim
Recent findings [1][2] in the synthesis and thermoelectric (TE) properties of bismuth selenide (Bi2Se3) nanoparticles on CNTs have inspired us to incorporate such CNT/Bi_2Se_3 hybrid structures in polymer-based nanocomposites. The promising TE properties of CNT/Bi_2Se_3 hybrid structures could greatly enhance the TE performance of flexible thermoelectric nanocomposites, which have so far fallen behind those of traditionally used inorganic materials.

Methods
Bi_2Se_3 nanostructures were synthesized on CNT networks via a catalyst-free vapour-solid deposition technique. [3] The obtained hybrid structures were solution-mixed or encapsulated into a non-conductive polymer matrix. The properties of the hybrid structures and nanocomposites were analysed by using scanning electron microscopy and energy dispersive X-ray analysis, a laboratory-made TE measurement setup as well as a physical property measurement system.

Results
In the presented work we measured the TE properties of two types of nanocomposites. One prepared by a more conventional approach of solution-mixing the TE hybrid filler and the other prepared by a more innovative way of encapsulating the CNT/Bi_2Se_3 hybrid networks in a polymer matrix. [4]

Conclusions
The properties of the solution-mixed and encapsulated polymer nanocomposites were compared. The encapsulation method is proven to be superior, requiring less TE hybrid structure material and producing nanocomposites with a higher TE power factor.

Acknowledgements
This work was funded by the European Regional Development Fund (ERDF) project no. 1.1.1.1/19/A/138

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CHEMICAL EXPOSURE AND ABRASION EFFECT ON PHOTOCATALYTICAL ACTIVITY OF ANTIBACTERIAL SURFACES COVERED WITH ACRYLIC MATRIX

Mati Kook [1], Ellen Leib [1], Kristjan Saal [2], Angela Ivask [3], Vambola Kisand [1]

[1.] Institute of Physics, University of Tartu,W. Ostwaldi Str. 1, 50411 Tartu, Estonia, [2.] University of Tartu, Institute of Physics, Estonia, [3.] Institute of Molecular and Cell Biology, University of Tartu, Riia 23, 51010 Tartu, Estonia

Keywords
antimicrobial coating; ZnO/acrylic coating

Actuality and aim
Bacterial infections are exerting a significant impact on public health, since microbial pathogens cause a higher burden to public health than either cancer or cardiovascular diseases. One effective way to prevent the spread of microbial pathogens is to stop their transmission from person to person or via cross-contaminated surfaces, e.g. using antimicrobial coatings.
Antimicrobial coatings are often evaluated only for their antibacterial activity and not for the effect of cleaning or wearing. The aim of the present work is to assess the effect of cleaning and wearing on the antibacterial multimodal ZnO/acrylic coatings which have also photocatalytic properties.

Methods
Photocatalytic activity measurements; XPS; AFM; SEM; surface abrasion tests; surface bleaching with NaOCl;

Results
UVA-induced photocatalytic activity of the ZnO/acrylic antimicrobial surfaces was measured before and after several cycles of chemical cleaning and mechanical wearing.
Two kinds of ZnO particles were used to fabricate ZnO/acrylic antimicrobial coatings – self-synthesized ZnO nanorods and industrial ZnO microparticles. Generally, photocatalytic activity of ZnO/acrylic antimicrobial surfaces were remained after chemical cleaning and mechanical wearing. Respective antimicrobial efficacy tests are in progress.

Conclusions
The UVA-induced photocatalytic activity of the ZnO/acrylic antimicrobial surfaces were remained after several cycles of cleaning and wearing.

MECHANICAL STABILITY OF MWCNT AND Bi_2SE_3 THERMOELECTRIC POLYMER COMPOSITE THIN FILMS

Lasma Bugovecka [1], Krisjanis Buks [2], Jana Andzane [3], Olesja Starkova [4], Juris Bitenieks [5], Janis Zicans [5], Donats Erts [3]

[1.] Institute of Chemical Physics, University of Latvia, [2.] SIA 3D Strong, 36 Institūta street, LV-2130, Ulbroka, Latvia, [3.] Institute of Chemical Physics, University of Latvia, Jelgavas street 1, LV-1004, Riga, Latvia , [4.] Institute for Mechanics of Materials, University of Latvia, Jelgavas str. 3, LV 1004, Riga, Latvia, [5.] Institute of Polymer Materials, Faculty of Materials Science and Applied Chemistry, Paula Valdena street 3/7, LV-1048 Riga, Latvia

Keywords
polymer nanocomposites, flexible thermoelectric films, bismuth selenide

Actuality and aim
Heat loss from many non-planar surfaces (industrial pipes, chimneys, human bodies) urges the development of flexible thermoelectric (TE) materials able to convert it to the useful energy [1]. Aim of this work was to test the mechanical and electrical stability of innovative flexible thermoelectric composite films where multi-walled carbon nanotube (MWCNT)-Bi_2Se_3 hybrid networks are combined with different polymers.

Methods
MWCNT-Bi_2Se_3 hybrid networks were prepared on a glass or polyimide film by consequent spray-coating and catalyst-free physical vapour deposition methods [2]. The stability and durability of the MWCNT-polymer and MWCNT-Bi_2Se_3-polymer films were tested performing uniaxial tensile tests, as well as bending tests while measuring film resistance and Seebeck coefficient using custom setup.

Results
MWCNT and MWCNT-Bi_2Se_3 networks were synthesised on flexible polyimide film surface, encapsulated in polyvinyl alcohol (PVA) or mixed in PVA. First two methods preserve the hybrid structures, but the mixing method breaks the bonds between hybrid structures [3]. The electrical resistance stability during 100 bending cycles down to 3 mm radius for different types of composites was analysed and compared. Additionally, dependence of elastic and strength properties of MWCNT-Bi_2Se_3 hybrid networks encapsulated in PVA on MWCNT content was studied [4].

Conclusions
MWCNT and MWCNT-Bi_2Se_3 polymer composite films showed great mechanical and electrical stability, proving their high potential for applications in flexible thermoelectrics.

Acknowledgements
This work was funded by the ERDF project No. 1.1.1.1/19/A/138.

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ROLE OF POLYMER TO FORMING OF FE_3O_4 /FE $_2TIO_5$ CORE-SHELL NANOFIBERS, DEPOSITED BY COAXIAL ELECTROSPINNING

Viktoriia Fedorenko [1], Roman Viter [1], Karlis Grundsteins [1], Arta Zarina [1], Agris Berzins [2], Viesturs Sints [3]

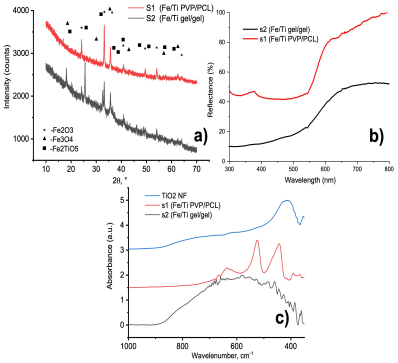
[1.] University of Latvia, Institute of Atomic Physics and Spectroscopy, Laboratory of Optical Biosensors and Functional Nanomaterials, [2.] University of Latvia, Faculty of Chemistry, [3.] University of Latvia, Institute of Physics

Keywords
metal oxides, core-shell nanofibers, coaxial electrospinning

Actuality and aim
Coaxial electrospinning is a novel technique for deposition of multicomponent nanofibers. Forming of core-shell nanostructures depends on many parameters, such as core-shell polymers, precursors, applied electrical field and collector rotation speed.
In the proposed research we report on development of Fe_3O_4/Fe_2TiO_5 core-shell nanofibers, deposited by coaxial electrospinning. Role of the polymers of core and shell to the final composition of the electrospun nanofibers was studied. Structure and optical properties of the core-shell nanofibers have been investigated and analyzed.

Methods
Iron nitrate (core) and Titanium isopropoxide (shell) were added to 10 and 8% solutions of Gelatin in Acetic acid (I). PVP:core in DMF and PCL shell in Chloroform (II) were also used for core-shell nanofibers synthesis for comparison analysis. Fe_2TiO_5/TiO_2 core-shell nanofibers have been deposited by coaxial electrospinning (20 (I)-21.4 (II) kV, 15 cm, 200 (I)-325 (II) rpm) and annealed at 600 °C for 2 hours.
Structure properties of the core-shell nanofibers have been investigated by XRD, SEM/EDX, FTIR and diffuse reflectance (300-800 nm)

Results
SEM images showed nanofibers of 500 nm in diameter and 4 micrometers lengths. XRD analysis identified magnetite Fe_3O_4 and hematite Fe_2O_3 (identical peak position are also for Fe_9TiO_{15}) phases. FTIR analysis showed the presence of Fe_2O_3 and Fe_3O_4 phases in the core material. Diffuse reflectance showed absorption bands at 2.3, 2.8, 2.5 and 2.2 eV (I) and 2.4, 2.5, and 2.1 eV (II). In case of using Gelatin polymer (I), we observed the increase of visible absorption.



a) XRD of Fe/Ti, b) Diffuse reflectance, and c) FTIR of Fe/Ti core-shell nanofibers

Conclusions
The choice of polymer defines structure, electronic and optical properties of the core-shell nanofibers.

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FE-NANOPARTICLE SEEDED GROWTH OF BI_2SE_3 NANORIBBONS

Andrei Felsharuk [1], Kiryl Niherysh [1], Edijs Kauranens [1], Gunta Kunakova [1], Davis Gavars [1], Jana Andzane [1], Krisjanis Smits [2], Igor Iatsunskyi [3], Donats Erts [1]

[1.] Institute of Chemical Physics, University of Latvia, Raina blvd. 19, Riga LV-1586, Latvia, [2.] Institute of Solid State Physics, University of Latvia, Kengaraga str. 8, Riga LV-1586, Latvia, [3.] NanoBioMedical Centre, AMU 61-614, Wszechnicy Piastowskiej str. 3 Poznan, Poland

Keywords
topological insulator, magnetic doping, physical vapour deposition

Actuality and aim
Topological insulators (TIs) attracted interest among researchers in the recent decade due to their unique band structure with gapless conducting surface states and insulating bulk. The surface states of TIs are protected by time reversal symmetry. Introducing of magnetic impurities in the TIs is a direct way to break this symmetry and to induce such effects as anomalous quantum Hall effect, which may have potential applications in future electronic devices [1].
The aim of this research is to develop a simple and robust method of introduction of magnetic dopants into bismuth selenide (Bi2Se3) nanoribbons.

Methods
A simple physical vapour deposition technique [2] was used for the growth of Bi_2Se_3 nanostructures on different substrates coated by the iron nanoparticles. Initial structural analysis of synthesized nanoribbons was performed using scanning electron and atomic force microscopies. Transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDX) technique and transport property measurements were used for more in-depth analysis.

Results
Various iron nanoparticles and Bi_2Se_3 nanoribbons parameters were inspected depending on initial Fe layer thickness. TEM and EDX data of the synthesized nanostructures verify the concentration of magnetic impurities in them up to 10 at %.

Conclusions
Demonstrated method of magnetic doping allows to obtain nanostructures with reliable dopant concentrations up to 10 at %.

Acknowledgements
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CALCULATED OPTICAL PROPERTIES OF CHALCOPYRITIC SOLID SOLUTIONS FOR PHOTOVOLTAIC APPLICATIONS

Jurij Grechenkov [1], Aleksej Gopejenko [1], Dmitry Bocharov [1], Anatoli Popov [1], Mikhail Brik [2], Sergei Piskunov [1]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Institute of Physics, University of Tartu, Estonia

Keywords
DFT, TDDFT, chalcopyrite, photovoltaics

Actuality and aim

Chalcopyrites are ternary semiconductor materials that have well-known applications in photovoltaics [1] as well as promising properties regarding non-linear optics [2] and scintillating behavior [3]. Although such compounds as CIGS have been studied in detail since 1980's [4] and have also found successful commercial applications [5], the search for a more efficient and cost-effective solar cell material continues. The present study aims to investigate alternative chalcopyritic compounds using computational methods with the hope of finding a good candidate for future use in photovoltaics.

Methods

The investigation is done using quantum-chemical computational codes such as CRYSTAL17, [6] Quantum Espresso [7] and Yambo [8]. A special care is given treating solid solutions that come up naturally when dealing with band gap tuning by altering the chemical composition of a given material. Optical properties are computed by the implementation of time-dependent density functional theory (TD-DFT). Different defects are also considered.

Results

Of all considered functionals for DFT computations HSE06 shows the best agreement with experimental results. The effect of atomic position in a crystallographic cell is shown to be negligible for chalcopyritic solid solutions. As a result of the modelling spectra were acquired with accuracy corroborated by comparison with data found in literature [6].

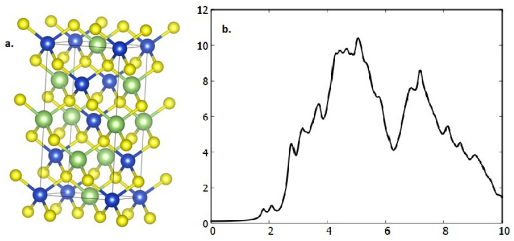


Fig. 1 a. – chalcopyrite crystal structure, b. – example of calculated spectra ($CuGaS_2$)

Conclusions

We created a novel model for chalcopyritic materials that can be used in a predictive fashion to study lesser-known chalcopyrites. Ongoing research concentrates on a wider variety of compounds and will serve as valuable input for experimentalists and manufactures alike.

Acknowledgements

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EFFECT OF THE CATIONS ON THE SEI LAYER FORMATION ON THE BI2SE3 ANODE IN AQUA MEDIUMS

Yelyzaveta Rublova, Vitalijs Lazarenko, Vanda Voikiva, Raimonds Meija, Jana Andzane, Donats Erts

Institute of Chemical Physics, University of Latvia

Keywords
Solid electrolyte interface; anodes; aqueous-based battery; current sources

Actuality and aim
The increased demand for chemical power sources have led to a renewed interest in the development of water-based batteries. Cathodes commonly used for non-aqueous electrolytes are also applicable in aqueous solutions [1], but the selection of a suitable anode for aqueous media is a difficult task. A possible anode material for aqueous batteries can be bismuth chalcogenides Bi_2X_3 (X = S, Te, Se) [2]. An important aspect in the design of anodes is understanding how the solid electrolyte interfacial layer (SEI) is formed. Here we investigate how the cation (Li^+, Na^+) affects the SEI layer formation on the Bi_2Se_3 anode in aqua media.

Methods
The electrochemical measurements were performed at room temperature with 3-electrode cell with 3 M Ag/AgCl as a reference electrode, Pt wire as a counter electrode, and a Bi2Se3 thin film on the glass substrate as a working electrode. 5 M $LiNO_3$ and 1 M $NaNO_3$ was used as an electrolyte. For investigation were used cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

Results
Cyclic voltammetry showed that the cation had no effect on the potential for the formation of the SEI layer on the surface of the investigated anodes. The EIS data showed that the resistance of the SEI layer gradually decrease during cycling for both Li+ and Na+, which may indicate the instability of the formed SEI layer.

Conclusions
Studies allow us to conclude that the mechanism of formation of the SEI layer on Bi_2Se_3 anode in aqua mediums for Li^+ and Na^+ is similar, the nature of the cation does not affect the formation of the SEI layer.

Acknowledgements
This work was supported by project No. 1.1.1.2/VIAA/4/20/694.

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DETERMINATION OF LIGHT ELEMENT CONTENT IN SODIUM BISMUTH TITANATE SAMPLES USING SECONDARY ELECTRON HYPERSPECTRAL IMAGING

Edgars Vanags, Marija Dunce, Liga Bikse, Annamarija Trausa, Krisjanis Smits

Institute of Solid State Physics, University of Latvia

Keywords
SEM, SEHI, elemental analysis, sodium bismuth titanate

Actuality and aim
Although scanning electron microscopes (SEM) are also equipped with energy-dispersive X-ray spectroscopy (EDX) detectors designed to analyze elements of samples, the EDX has its own drawbacks. The EDX analysis can be destructive due to the high-speed voltage of electrons required to excite a sample, as well as the determination of the elemental composition of samples in the case of light elements (LE) introduces errors in the results, or even their detection is impossible. LE detection is also problematic by using other classical LE detection methods. There is a strict need for an alternative analysis of LE for the manufacturing of electronic devices and their quality control [1].
Although studies have been performed using secondary electron hyperspectral imaging (SEHI) for various materials, no automated algorithm and an optimal combination of microscope/detector settings and parameters have been developed to make the method feasible for analysis of LE in the scanning electron microscope.

Methods
SEHI, by applying various electron detectors, such as: through the lens detector (TLD), ion conversion and electron (ICE) detector, and Everhart–Thornley detector (ETD), and the various microscope and detector parameters was used for the examination of LE in sodium bismuth titanate (SBT) materials. The obtained SEHI results was compared with the results of other element detection methods.

Results
An automated data acquisition script was created and the described method was used to study the stoichiometry of SBT samples.

Conclusions
The SEHI approach shows promising elemental analysis results as a non-destructive LE determination method in nanomaterial science.

Acknowledgements
The financial support of the project "SJZ/2021/06" is gratefully acknowledged.

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SERS SUBSTRATES BASED ON GOLD NANOPARTICLE-COATED ZNO TETRAPODS

Annamarija Trausa, Ingars Lukosevics, Liga Bikse, Edgars Vanags, Edgars Butanovs, Krisjanis Smits

Institute of Solid State Physics, University of Latvia

Keywords
ZnO tetrapods, SERS substrates, SERS, preparation methods

Actuality and aim
SERS (surface-enhanced Raman scattering) is a powerful tool for ultra-sensitive vibrational spectroscopy that is being extensively studied [1]. Because of the excitation of collective electron oscillations called surface plasmon resonance, low-dimensional metal nanoparticles like Au have distinctive optical features in the visible spectrum region [2]. However, challenges in fabricating highly uniform nanostructures at low cost, instability issues such as easy aggregation and oxidation during the application, and a limited number of noble metals with excellent SERS activity have hampered the development and widespread use of these noble metal substrates. Due to their advantages over noble metals, semiconductors such as ZnO also have steadily been used as one of the important SERS substrates [3].

Methods
ZnO tetrapods were applied to the surface of two different substrates. 10x10 mm samples were infused with gold nanoparticles and one series of samples was treated with Rhodamine B. Au-coated ZnO nanostructures were analysed by scanning electron microscopy and Raman spectroscopy.

Results
Different types of ZnO Au structured films were prepared and their SERS efficiency was compared. Most efficient structures and optimal ZnO and Au concentrations were found.

Conclusions
Our current results suggest that ZnO tetrapod substrates and Au nanoparticle-coated ZnO tetrapod substrates improve SERS activity and therefore can be used as cheap and efficient SERS-active substrates. Moreover, possible ways of ZnO arrangements could further increase the efficiency.

Acknowledgements
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OPTIMAL SYNTHESIS PARAMETERS AND CHARACTERIZATION OF CATALYST-FREE GROWN Bi_2SE_3 NANORIBBONS

Didzis Salnājs [1], Raitis Sondors [2], Jana Andžāne [2], Donāts Erts [2]

[1.] Institute of chemical physics, University of Latvia, [2.] UL Institute of chemical physics

Keywords
Bi_2Se_3, PVD, nanoribbons

Actuality and aim
Bi_2Se_3 is a narrow gap semiconductor, which has been widely studied for infrared detectors and has demonstrated potential for application in photochemical and thermoelectric devices, furthermore, this material belongs to a novel class of 3D topological insulators that are insulating in bulk and host Dirac states on its surfaces. Surface state properties, such as spin-momentum locking, make TIs attractive for potential applications in dissipationless electronics and spintronics. However, access to these peculiar properties of the surface states is disrupted by the conductance from the material bulk resulting from unintentional doping [1].

Methods
Currently available Au catalyzed physical vapor depositon (PVD) and catalyst-free PVD methods for the synthesis of high-quality TI nanowires are limited by the growth mechanism from Au nanoplate seeds and other factors, leading to the growth of nanoribbons with thickness above 30 nm [2,3] . To ensure an increase in the surface-to-volume ratio of bulk-free 3D TI nanoribbons, thus reducing their thickness without affecting material quality and purity, a catalyst free PVD synthesis method was chosen.

Results
Atomic force microscopy (AFM) was used to measure the nanowire thickness and surface roughness as well as compared as a function of the adjusted synthesis parameters. A controllable reduction of mean nanoribbon thickness was achieved without degradation of the nanoribbons' surface roughness. Scanning electron microscopy (SEM) was used to characterize the nanostructure morphology and physical dimensions.

Conclusions
By adjusting the catalyst-free PVD synthesis method, a successful reduction of mean nanoribbon thickness was achieved.

Acknowledgements
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TOWARDS SURFACE-ENHANCED RAMAN SPECTROSCOPY ON THE TIP OF OPTICAL FIBER: COMPARISON OF SUBSTRATES

Liga Bikse, Edgars Vanags, Annamarija Trausa, Krisjanis Smits

Institute of Solid State Physics, University of Latvia, Latvia

Keywords
SERS, FIB-SEM, optical fiber

Actuality and aim
An enhancement in Raman signal intensity can be achieved by using electromagnetic and chemical surface properties, resulting in surface-enhanced Raman spectroscopy (SERS) [1]. The nanostructured pattern style arrangements and particle size play the critical role in Raman signal enhancement. One of the possible ways to prepare them is to use a focused ion beam (FIB) and it gives a relatively fast way to test different SERS substrate patterns. Optical fiber is ideal for its mobility and light transmission, thus producing nanostructures on its tip could lead to applications in biomedicine [2]. Therefore, the aim of the work is to study suitable materials and designs for nanostructure fabrication on the optical fiber's tip for SERS applications and comparison with semiconductor-metal substrates.

Methods
Two substrate types, metal-dielectric (gold-glass) and metal-semiconductor (gold-silicon) were used as surfaces for SERS substrate production. 40 nm thick gold layer was sputtered onto glass and silicon. The gold nanostructures were etched as squares of different sizes by a FIB in a scanning electron microscope. Rhodamine B was employed as the Raman active molecule. Raman scattering was excited with the 785 nm laser and spectra were obtained with a Raman spectrometer, equipped with an optical microscope.

Results
Obtained results contain the recommendation for optimal optical fiber SERS substrate and nanostructure combination.

Conclusions
FIB can be used to produce SERS substrates and metal film preparation plays a crucial role in SERS efficiency.

Acknowledgements
The authors gratefully acknowledge the financial support of the ERDF project Nr. 1.1.1.1/21/A/053 realized at the Institute of Solid State Physics, University of Latvia.

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SERS-ACTIVE SUBSTRATES BASED ON SILVER NANOPARTICLE ARRAY INDUCED SURFACE LATTICE RESONANCE

Nadzeya Khinevich [1], Asta Tamulevičienė [2], Mindaugas Juodėnas [3], Tomas Tamulevičius [2], Sigitas Tamulevičius [2]

[1.] Institute of Materials Science Kaunas University of Technology, Lithuania, [2.] Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59 LT-51423 Kaunas, Lithuania ; Department of Physics, Kaunas University of Technology, Studentų St. 50, Kaunas LT-51423, Lithuania; UAB Nanoversa, K. Baršausko St. 59 LT-51423 Kaunas, Lithuania , [3.] Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59 LT-51423 Kaunas, Lithuania ; Physics Department, Chalmers University of Technology, Gothenburg 41296, Sweden

Keywords
SERS, SLR, silver nanoparticles

Actuality and aim
Silver nanoparticles of various sizes and shapes are widely used to fabricate SERS substrates due to their strong light absorption and scattering properties in the visible range. When nanoparticles form an array, the effect of surface lattice resonance appears. The study aims to show that by changing the size of silver nanoparticles while maintaining the same array periodicity, the position of the SLR peak can be overlapped with different excitation laser wavelengths, providing maximum SERS substrate sensitivity.

Methods
Monodisperse spherical silver nanoparticles were synthesized using seed mediated growth as described in [1]. Deposition of synthesized nanoparticles in the trapped PDMS template was carried out by Capillary assisted particle assembly (CAPA) [2]. SERS measurements of 2-naphthalenethiol (2NT) were performed using a multiwavelength Raman microscope equipped with 473 nm - 785 nm excitation wavelengths. The simulation of the prepared substrate's transmittance and absorbance spectra, and electromagnetic field distribution was done using COMSOL multiphysics software.

Results
The highest intensities of SERS-spectra were registered when the position of the SLR peak overlapped with a specific excitation wavelength via changing the deposited silver nanoparticle size. Experimental results were verified by computer simulations.

Conclusions
The presented method of SERS active substrates fabrication, based on the SLR effect, has shown its effectiveness in creating substrates with the required plasmonic properties and can be widely used for SERS applications.

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IMPACT OF ELECTRODES ON PROPERTIES OF FLEXIBLE ENCAPSULATED Bi_2SE_3/CNT HYBRID NETWORK MATERIALS

Loreta Brauna [1], Krisjanis Buks [1], Jana Andzane [2], Michael Katkov [3], Donats Erts [2]

[1.] 3D Strong Ltd., Ropazu nov., Ulbroka, Instituta iela 36-17, LV-2130 ; Institute of Chemical Physics, University of Latvia, Jelgavas iela 1, Riga, Latvia, LV-1004, [2.] Institute of Chemical Physics, University of Latvia, Jelgavas iela 1, Riga, Latvia, LV-1004, [3.] 3D Strong Ltd., Ropazu nov., Ulbroka, Instituta iela 36-17, LV-2130

Keywords
Bismuth selenide, carbon nanotubes, polyvinyl alcohol, chemical vapor

Actuality and aim
The development of efficient thermoelectric composites is increasing due to their promising potential applications in flexible thermoelectric (TE) devices.[1] An alternative to electrically conductive polymers is non-conductive polymers, and one way to prepare a composite is to combine CNT-Bi_2Se_3 with a non-conductive polymer to fabricate n-type flexible TE films. Two ways to do this: use filler [2] or use encapsulation.
Good quality electrodes are important for the encapsulation to preserves the electrical contacts established in the CNT-Bi_2Se_3 network.

Methods
PVA-Bi_2Se3/CNT flexible films with different types of electrical contacts have been fabricated. Spray-coating method is used to prepare CNTs networks. To synthesize Bi_2Se_3 nanostructures, the chemical vapor deposition was used. The TE properties and morphology of the fabricated composite films were characterized using scanning electron microscopy, energy dispersive X-ray spectroscopy and laboratory-made TE measurement setup.

Results
PVA-Bi_2Se_3/CNT flexible films with different types of electrical contacts (gold coated copper pins, silver paste) have been fabricated. The Seebeck coefficient and resistance of Bi_2Se_3-MWCNT hybrid networks before and after encapsulation in PVOH is measured.

Conclusions
The application of the electrodes to the network before the encapsulation is necessary to avoid high contact resistance with the measurement electrodes and unwanted energy dissipation in the contact areas.
The increase of Seebeck coefficient up to 40% was observed as the encapsulation was provided with electrodes while increasing resistance of the samples by 2-25%.

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APPLICATION OF GRAPHENE FOR ENHANCEMENT OF PHYSICAL PROPERTIES OF BI_2SE_3 AND BI2SE3/ZNO NANOSTRUCTURES

Margarita Baitimirova [1], Jana Andzane [1], Roman Viter [2], Mikhael Bechelany [3], Donats Erts [1]

[1.] Institute of Chemical Physics, University of Latvia, [2.] Institute of Atomic Physics and Spectroscopy, University of Latvia, [3.] European Institute of Membranes, University of Montpellier, CNRS, France

Keywords
graphene, bismuth selenide, zinc oxide, thermoelectric, photoluminescence

Actuality and aim
The combination of graphene (G) – unique 2D carbon nanomaterial – with other nanomaterials can provide creation of layered nanostructures with improved physical properties. Enhancement of properties is predicted to arise from the changes in crystal structure of nanostructures during their synthesis on G substrates [1, 2], and due to the charge transfer at the inner interfaces of the of created layered structures [3].

Methods
Chemical vapor deposition, physical vapour deposition [4] and atomic layer deposition were used for the synthesis of G, bismuth selenide (Bi_2Se_3) and zinc oxide (ZnO) respectively. Morphology and structure of the samples were characterized using scanning electron microscopy, atomic force microscopy and X-ray diffractometry. Thermoelectric (TE) measurements were performed for Bi_2Se_3 in G/Bi_2Se_3/G layered structures using custom setup. Photoluminescence of ZnO in G/Bi_2Se_3/ZnO heterostructures was measured by fiber optics spectrometer with excitation wavelength 266 nm and compared with quartz/Bi_2Se_3/ZnO and ZnO nanolayers with the same thickness.

Results
Correlation between the structure, optical and TE properties of semiconductor nanolayers in layered nanostructures is analyzed. Possible mechanisms of impact of G substrates on the properties of layered nanostructures and potential ways for improving the optical and TE properties of graphene-containing layered nanostructures are proposed.

Conclusions
Fabricated G/Bi_2Se_3/G and G/Bi_2Se_3/ZnO layered structures are perspective materials for applications, respectively, in TE and optoelectronic devices.

Acknowledgements
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THE TECHNOLOGICAL FEATURES OF NANOSTRUCTURES FORMATION ON THE SURFACE OF INDIUM PHOSPHIDE BY ELECTROCHEMICAL ETCHING

Yana Suchikova [1], Yana Suchikova [1], Ihor Bohdanov [1], Sergii Kovachov [1], Andriy Lazarenko [1], Aleksandra Moskina [2], Tamara Tsebriienko [2], Anatoli Popov [2]

[1.] Berdyansk State Pedagogical University, Ukraine, [2.] Institute of Solid State Physics, University of Latvia

Keywords

electrochemical etching, indium phosphide, porous semiconductors

Actuality and aim

In recent years, the porous structures of semiconductors have attracted a fairly high scientific and technological interest due to their different optical and electrical properties [1]. InP is a III-V semiconductor with much higher electron mobility than, for example, silicon and can used in high-power and high-frequency optoelectronic devices. Electrochemical methods for producing porous InP have a number of advantages, such as low processing temperature, low damage, low cost and versatility [2].

The purpose of this work is to reveal the mechanism of formation of a porous layer on the surface of a single-crystal of indium phosphide by etching.

Methods

At first, grinding and polishing were used to give the structural perfection for samples surface. Then the chemical polishing was applied in a mixture of acids.

Electrochemical etching of the crystals was carried out in an aqueous-alcoholic solution of hydrofluoric acid.

Results

Using the SEM method, it was found that no pores were formed on the surface of p-type InP under current density 150-200 mA/cm2 and etching time 10-20 min.

The current-oriented pores are formed on the surface of n-InP (100) crystals. They grow deep into the crystal in mutually parallel cylinders with a slight rounding of the bottom pore. It is not possible to obtain chain and crystallographically oriented pores on surfaces (100).

The nanostructures obtained on the surface of n-InP (111) consists of two sets of "111" crystallographically oriented pores that intersect with each other forming channels, tracks, and chains. Tracks have lengths from 1 to 5 microns and cross-sectional size from 100 to 200 nm.

Conclusions

Thus, it was shown that the morphology of the samples will depend on the type of conductivity of the original crystal.

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INFLUENCE OF FEMTOSECOND LASER PARAMETERS FOR IMPOSING LASER-INDUCED PERIODIC SURFACE STRUCTURES ON SILICON SURFACE

Mantas Mikalkevičius, Tomas Tamulevičius, Asta Tamulevičienė

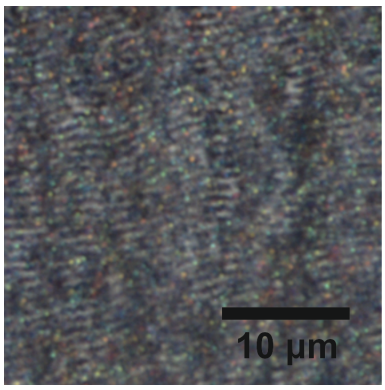
Institute of Materials Science of Kaunas University of Technology, K. Baršausko Str. 59, LT-51423, Kaunas, Lithuania

Keywords
femtosecond laser, LIPSS, silicon

Actuality and aim
Processing of solids near their ablation threshold by high intensity polarized laser irradiation may lead to the development of regular nanoscale structures known as Laser-induced Periodic Surface Structures (LIPSS). Applying LIPSS to a surface can lead to numerous applications of surface functionalization including but not limited to improved wetting performance [1], antibacterial activity [2], and low optical reflectance [3]. This work aims to find the optimal femtosecond laser processing conditions for periodic structure formation on the silicon wafer surface.

Methods
In this work, the fundamental harmonic (1030 nm) of a linearly polarized Yb:KGW femtosecond laser (Pharos, Light Conversion) was used. The pulse density and average power was varied from 500 to 1500 p/mm and from 38 to 190 mW respectively. N-type 100 orientation silicon wafers were used as substrates. Periodic structures were analyzed by the dark-field optical microscope (Olympus).

Results
When the laser power was less than 114 mW periodic structures were not formed. Over 114 mW one starts to see laser modification on the surface, but it is clearly visible only when 152 mW power is applied. If the power is higher than 152 mW the structures become melted and no longer have a defined shape. Also, the proper pulse density or pulse overlap has to be selected. We noticed that using 200 kHz repetition rate and 800 p/mm pulse density a good value for continuous structure formation



Optical microscope micrograph of silicon surface with LIPPS after the laser treatment

Conclusions
In this work, we have demonstrated that it is possible to impose self-organized periodic structures on semiconductors using a femtosecond laser. The optimal conditions for periodic structure formation using investigated laser micromachining system are power – 152 mW, pulse density – 800 p/mm.

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TOPOLOGICAL DEFECTS MOVEMENT CONTROL IN LIQUID CRYSTAL CELLS

Pavlo Golub, Mikhail Vasnetsov [1]

Institute of Physics NAS of Ukraine

Keywords
liquid crystal, Topological defects, Disclination.

Actuality and aim
We report the series of the experiments which main aim was the visualization of a topological defect i.e. making it visible with naked eye, and control its movement through the photoalignment.

Methods
For the visualization of the disclination movement in the LC cell in a real time the cell where filled with the LC doped with the pigment red nanoparticles. They have aggregated in the disclination which make it well visible with the naked eye.
To move the disclination the test photosensitive substrate where irradiated by the 532 nm laser light which caused the reorientation of the director on the test substrate and, as a result, to changing the position of the disclination in a LC bulk.

Results
The results of the theoretical and experimental results showed that irradiation of the photosensitive surface causes the modulation of the easy axis on the photosensitive surface and, as a result cause director reorientation on the photosensitive surface.

Conclusions
The director orientation in the bulk depends on orientation on the substrates so the disclination position depends on orientation on the surface. Irradiation of the photosensitive causes rotation of the disclination and the angle of the rotation depends on dose.

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THERMOELECTRIC PROPERTIES OF COPPER OXIDE NANOWIRE NETWORKS

Davis Gavars [1], Raitis Sondors [2], Jana Andzane [2], Donats Erts [2]

[1.] Institute of Chemical Physics, Latvia, [2.] Institute of Chemical Physics

Keywords
nanowire network, copper oxide, thermoelectric device

Actuality and aim
The thermoelectric effect of nanostructured materials has been the focus of many studies. Most commonly nanostructures obtained using toxic elements, such as bismuth and lead, are used in such research. [1] Much safer and cheaper materials with similar properties are copper oxides. Copper oxide is non-toxic, cheap, eco-friendly, and a widely available p-type semiconductor, which may be a good alternative for use in thermoelectric devices.

Methods
Copper oxide nanowires were synthesized via thermal oxidation of copper [2] and used to fabricate nanowire networks, which were then reduced. Scanning electron microscopy (SEM) equipped with an energy-dispersive X-ray diffraction (EDX) system was used to characterize the morphology and chemical composition of the nanowires. The electrical conductivity and thermoelectric properties of the sample were characterized using a custom setup.

Results
The annealing of copper oxide nanowires significantly improves the Seebeck coefficient, as well as electrical conductivity. Possible mechanisms underlying such improvement of properties are discussed.

Conclusions
Copper oxide nanowire networks can be successfully obtained by thermal oxidation and further annealing improves their potential for thermoelectric applications.

Acknowledgements
This work is funded by the ERDF project No. 1.1.1.1/20/A/144.

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REACTIVE E-BEAM EVAPORATION OF YTTRIUM: A SPECTRAL AND STRUCTURAL INVESTIGATION OF THE GROWTH KINETICS

Halil Arslan [1], Ilze Aulika [1], Inga Pudza [1], Anatoly Sharakovsky [1], Līga Bikse [1], Martins Zubkins [1], Georgi Chikvaidze [1], Juris Purans [1]

[1.] Institute of Solid State Physics, University of Latvia

Keywords

e-beam evaporator, yttrium, growth dynamics

Actuality and aim

Being the fact that the structural evaluation stays still uncertain, yttrium based oxyhydride thin films are the one of the most promising candidate with photochromic behaviour. In contemplation of the understanding/constructing, as regards the scope of this research, the relation between crystal arrangements and spectroscopic response; yttrium, yttrium oxide and yttrium oxyhydride thin films were deposited by e-beam evaporator

Methods

E-beam evaporator, XRD, XPS, XAS

Results

The results obtained from X-ray diffraction reveal: a- the formation of Y metal is accompanied by monoclinic yttria, b- fully oxidized yttrium may form x-ray amourphous structure, c- hydrogen may trigger crystal formation. XPS measurements demonstrate the fully oxidized yttrium is the most stable phase and even at very low oxygen partial pressure levels yttrium captures the oxygen around during the film formation. In addition to that XAS (and XPS) measurements illustrates yttrium has unusual valencey in the presence of hydrogen in YHOx structure.

Conclusions

This study set out to determine the formation dynamics of yttrium hydrides (oxyhydrides). One of the most significant findings gained from this study is yttrium has unusual oxidation state in hydride/oxydride structure. The second finding is the development of the monoclinic phase yttria is concurrent with alpha phase yttrium evolution. The third major outcomes obtained from this study is the Y3d binding energy shows diversity depending on the crystal structure for the same oxidation state.

Acknowledgements

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EFFECT OF THERMALLY DEWETTED AU NANOPARTICLES ON THE MORPHOLOGY OF BI2SE3 NANORIBBONS SYNTHESIZED BY PHYSICAL VAPOR DEPOSITION

Raitis Sondors, Gunta Kunakova, Jana Andzane, Edijs Kauranens, Liga Jasulaneca, Donats Erts

Institute of Chemical Physics, University of Latvia

Keywords
Bi_2Se_3, nanoribbon, physical vapor deposition, morphology, Au nanoparticles

Actuality and aim
Bismuth selenide (Bi_2Se_3) is a semiconducting material that belongs to the 3D topological insulator class. In order to utilize the topological surface states Bi_2Se_3 nanoribbons [1], synthesis methods with tunable nanoribbon morphology must be developed.

Methods
Bi_2Se_3 nanoribbons were synthesized with physical vapor deposition (PVD) [2] on a thermally dewetted Au layer in a tube furnace. Au layers of various thicknesses were dewetted in order to obtain nanoparticles. Scanning electron microscopy was used to determine nanoribbon length and width distribution. Atomic force microsopy was used to determine nanoribbon thickness distribution. A physical property measurement system (PPMS) was used to determine nanoribbon electrical properties. X-ray diffraction (XRD) spectra were obtained to determine the dominating growth mechanisms.

Results
Length, width and thickness distributions of synthesized Bi_2Se_3 nanoribbons show that their morphology can be affected by the size of Au nanoparticles. Analysis of XRD spectra suggests that changing the size of Au nanoparticles affects the dominant growth mechanism of Bi_2Se_3 nanoribbons. PPMS measurements show Shubnikov-de Haas oscillations at a temperature of 2 K.

Conclusions
Changing the size of Au nanoparticles in a PVD sythesis can be used to control the morphology and growth mechanism of Bi_2Se_3 nanoribbons [3]. The electron transport properties of the Bi_2Se_3 nanoribbons are not degraded by the use of Au nanoparticles.

Acknowledgements
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OPTIMIZATION OF CONDITIONS FOR TESTING THE EFFICACY OF ANTIMICROBIAL SURFACES

Harleen Kaur, Merilin Rosenberg, Vambola Kisand, Angela Ivask

[1.] University of Tartu, Estonia

Keywords
Antimicrobial, surfaces, Escherichia coli, Staphylococcus aureus

Actuality and aim
The growing interest towards the use of non-antibiotic antimicrobials, for hygiene purposes has been evidenced by the increased level of current research. There is also a growing trend towards antimicrobials surface coatings. The two main key properties of antimicrobial surface coatings are activity towards the target microbes and safety against non-target species. Here, our goal is to clarify the differences in apparent efficiency of antimicrobial surfaces when analyzed using different test methods.

Methods
We varied three important test conditions during antibacterial analysis: air humidity, exposure media and bacterial drop-size.
We selected 99.9% solid copper as the model antibacterial surface and Escherichia coli (ATCC 8739) as the model bacterium while glass and stainless-steel surfaces were used as negative control surfaces. We will also test their antifungal activity against Candida albicans CAI4.
The surfaces were tested at high (90%), moderate (50%), and low (20%) RH conditions in different bacterial drop sizes (1x 50 µl and 5x 2 µl) in both organic rich exposure medium ("soil load") and oligotrophic (1:500 times diluted nutrient broth) medium to mimic the real life conditions.

Results
Initial results showed that all the varied parameters affected the antimicrobial efficiency of copper surfaces towards E.coli.

Conclusions
The lowest efficiency was obtained with large drop size and organic rich medium in 90% RH and the highest efficiency was observed for smaller drop size in oligotrophic exposure medium. The tests for other RH are yet to be performed.

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EVALUATION OF ANTIBACTERIAL PROPERTIES OF CU-DOPED TITANIUM DIOXIDE USING DFT CALCULATIONS

Elina Neilande [1], Yin-Pai Lin [1], Siarhei Zavatski [2], Hanna Bandarenka [2], Anatoli I. Popov [1], Sergei Piskunov [1], Dmitry Bocharov [1]

[1.] Institute of Solid State Physics, University of Latvia, Kengaraga 8, Riga, Latvia, [2.] Belarusian State University of Informatics and Radioelectronics, P.Brovka St., Minsk, 220013, Belarus

Keywords
Titanium dioxide, antibacterial properties, DFT, absorption spectrum

Actuality and aim

Antibacterial properties of materials have been studied for decades and recently they have been researched with new intensity, including antibacterial properties of solid-state materials. One of prospective materials with antibacterial properties is titanium dioxide (TiO_2). All three polymorphs of TiO_2 - anatase, rutile and brookite - have antibacterial properties [1], however research has shown that the most pronounced they are in anatase [2]. TiO_2 is a photocatalyst with a band gap > 3.2eV [2, 3]. Many harmful organic compounds can be destroyed by irradiating TiO_2 with UV or sunlight [2-6]. Doping TiO_2 with copper has been shown to improve its antibacterial properties even several times by increasing the properties of photocatalysis [7-9].

Methods

Calculation of both Cu-doped TiO2 bulk phase and its surface reactivity were performed using the ab initio computer modelling methods based on quantum chemistry and density functional theory (DFT) using CRYSTAL17 computer code [10]. Besides, the absorption spectrum was predicted by the GPAW code [11] for understanding the discrepancy between Cu-doped and pure TiO_2 bulk.

Results

A series of calculations were carried out to clarify how and whether doping with Cu affects the antibacterial properties of TiO_2. For the excited state simulations, real time time-dependent DFT is utilized to calculate the abs orption spectrum and to analyze the transition contribution for the doped Cu.

Conclusions

Ongoing research includes the use of other dopants, as well as the use of other methods for theoretical and experimental investigations of the material.

Acknowledgements

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IN-SITU OPTICAL CONTROL OF NANOPOROUS ALUMINA LAYER THICKNESS

Aleksandrs Dutovs, Vladislavs Perkanuks, Irina Oliševeca, Aušrinė Jurkevičiūtė, Raimonds Poplausks , Donats Erts, Juris Prikulis

Institute of Chemical Physics, University of Latvia

Keywords
porous alumina, nanotechnology, nanooptics

Actuality and aim
Classic method of producing porous alumina is two-step anodization, developed by Masuda et al. [1] This method allows to acquire hexagonal vertically aligned aluminium oxide nanopores which greatly serves as a template for producing dense nanoparticle arrays with high surface-to-volume ratio [2]. Thickness of nanoporous alumina layer directly depends on anodization time, however its control over time is not precise and afterwards requires damaging the sample for analysis of cross-section in SEM. In this study we report about all-optical non-damaging and non-invasive determination of porous layer thickness.

Methods
Porous alumina was synthesized by two-step anodization from high-purity aluminium and oxalic acid solution in water as an electrolyte [2]. During anodization process, sample was exposed to visible light and reflected light was collected. Calculated reflectance was compared to mathematical model where light interaction in multi-layered structure was simulated using aluminium, alumina, and electrolyte optical constants [3].

Results
We have achieved mostly linear relation between porous alumina layer thickness and anodization time (fig. 1) and our developed thickness control method demonstrates sufficiently high accuracy. Comparison of optically determined final porous alumina thickness value with ellipsometry results showed only slight deviation.

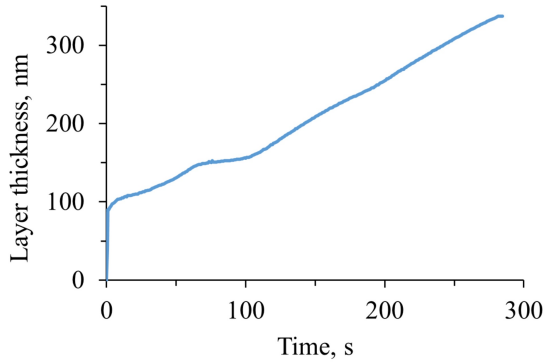


Fig.1. Relation between porous alumina layer thickness and anodization time

Conclusions
Method, demonstrated in this study, shows possibility for in-situ optical control of nanoporous alumina layer thickness without damaging sample and terminating anodization process when required thickness is reached.

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SENSING OF VASCULAR ENDOTHELIAL GROWTH FACTOR-A USING CLOSE PACKED AU NANOPARTICLE ARRAYS ON POROUS ANODIC ALUMINUM OXIDE-AL TEMPLATES.

Uldis Malinovskis [1], Amanda Reķe [1], Raimonds Poplausks [1], Aleksandrs Dutovs [1], Donats Erts [1], Indrikis Muiznieks [2], Juris Prikulis [1]

[1.] Institute of Chemical Physics, University of Latvia, [2.] Faculty of Biology, University of Latvia

Keywords

self-organized templates, VEGFA, optical biosensing, porous anodic aluminum

Actuality and aim

Vascular endothelial growth factor-A (VEGFA) is a multi-functional cytokine with important roles in normal and pathological angiogenesis [1]. Elevated levels of VEGFA are associated with many diseases, e.g., cancer, diabetic retinopathy, neovascular age-related macular degeneration and others [2-5]. Therefore, VEGFA is an important biomarker for different diseases.

In our study we tested the usability of plasmonic Au nanoparticle arrays (NA) on self-organized porous anodic aluminum (PAAO)-Al templates for refractometric detection of most abundant human VEGFA isoform – VEGF165.

Methods

Thin PAAO layer on Al surface with pore dia. ~40 nm and interpore distance ~110 nm was prepared using two-step anodization method[6]. Au NA on PAAO/Al templates were produced by capillary force assisted deposition of 60 nm dia. Au colloid suspension [7]. The obtained Au NA were functionalized with anti-VEGFA aptamer SL2B (5′-CAATTGGGCCCGTCCGTATGGTGGGT-SH - 3′) [8]. Dark-field micro-spectroscopy was done using fiber coupled spectrometer and halogen light source.

Results

The obtained plasmonic structures vary from dense, non-touching NA to randomly distributed nanoparticles. The produced Au NA have a strong scattering in the visible spectral range. After functionalization with DNA and subsequent treatment with BSA, Au NA were used for the detection of VEGF165 protein. Change of intensity of light scattering and shift of scattering maxima wavelength was detected at presence of 0.5 – 1 ng/ml VEGF protein.

Conclusions

Au NA on PAAO-Al templates are suitable substrates for optical detection of elevated concentrations of VEGFA protein.

The detection limit of our optical biosensor based on functionalized Au NA was 0.5 ng/ml.

Acknowledgements

Project identification No. 8.2.2.0/20/I/006

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LUMINESCENCE, XPS AND RAMAN OF CRYSTALLINE QUARTZ AFFECTED TO HIGH PRESSURE BY DETONATION

Anatolijs Truhins [1], Jevgenijs Gabrusenoks [1], Anatolijs Sarakovskis [1], Rudolf Mashkovtsev [2]

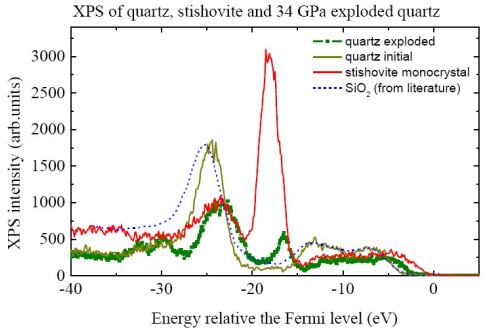
[1.] Institute of Solid State Physics, University of Latvia, [2.] Sobolev Institute of Geology and Mineralogy, Novosibirsk, Russia

Keywords
silicon dioxide, quartz, stishovite, detonation, luminescence, Raman, XPS

Actuality and aim
polymorphism of silicon dioxide under pressure with use of detonation

Methods
The spectra of Raman, X-ray photoelectron spectroscopy (XPS) and the spectra of X-ray excited luminescence of crystalline quartz samples subjected to different levels pressure by mean of detonation were compared with the spectra of the initial samples.

Results
The luminescence of a self-trapped exciton, which, when excited by X-rays has a high energy yield (~20%) in crystalline quartz, was analyzed in those samples. The deviations of the luminescence spectrum relative to unirradiated samples are small in the pressure range from 9 to 27 GPa. This means the preservation of quartz crystals in samples that are visually very different from optically transparent unexposed samples. A sharp change in the spectrum occurs for a sample subjected to a pressure of 34 GPa. The STE band practically disappeared and a band appeared at 350 nm. This band manifests itself in thermally stimulated luminescence (in contrast to the STE band, which is not observed at all in the TSL) and, therefore, can be attributed to some defects that have arisen due to the high pressure. This luminescence is not similar to the luminescence of a stishovite single crystal, however analyzes of XPS spectra allow assume some quantity of stishovite creation in the subjected to explosion samples. In the Raman spectra, which become very broad, the only sharp line at 466 cm-1, characteristic of α-quartz, was observed in the samples after pressure for remaining small crystals. This line strongly decreased for the sample subjected to a pressure of 34 GPa.



Comparison of XPS of quartz sample, subjected to high pressure (34 GPa) through detonation.

Conclusions
High pressure due to detonation leads to transfomation of crystalline quartz to amorphized stishovite.

Acknowledgements
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INFILTRATION CONTROL OF HIGHLY ORDERED NANOPOROUS ALUMINUM OXIDE MEMBRANES WITH AQUEOUS ELECTROLYTES

Valerii Malyshev [1], Irina Oliseveca [1], Raimonds Poplausks [1], Raimonds Meija [1], Ievgen Nedrygailov [2], Justin Holmes [3], Donats Erts [1]

[1.] Institute of Chemical Physics, University of Latvia, [2.] University Colledge Cork, Ireland, [3.] University Colledge Cork

Keywords

PAAO, porous anodic aluminium oxide, electrochemical impedance spectroscopy

Actuality and aim

Nowadays highly ordered porous anodic aluminum oxide (PAAO) is one of the frequently used platforms for a variety of applications:as templates for different nanostructures, for molecular separation, sensing, energy generation and storage [1].Effective impregnation of membrane pores with an electrolyte is of utmost importance in the electrochemical application of PAAO membranes.

Methods

Nanoporous anodic aluminum oxide layers with different pore diameters and different thicknesses have been prepared by the standard two-stage scheme anodization of electropolished aluminum sheet in 0.3 M oxalic or sulfuric acid with subsequent removal of the barrier layer. Free-standing PAAO membranes were obtained by subsequent etching of the aluminium layer. As the result, membranes with thicknesses of 9-112 μm were fabricated. The pores' diameters of the PAAO membranes obtained by anodizing in sulfuric acid were 13-20 nm and the diameters of the PAAO membranes obtained in oxalic acid were 33-40 nm.

Results

The average values of pore diameters, inter-pore distances, porosity and thickness of PAAO were measured by the processing of scanning electron microscopy images.

Conclusions

For PAAO membrane's pore infiltration electrolyte wetting, vacuum impregnation, pressure impregnation and lowering of surface tension of electrolyte solution with surface-active agents were used. The filling power of each technique was determined by using electrochemical impedance spectroscopy with a subsequent fitting of the obtained spectra.

Acknowledgements

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EXAFS STUDY OF NIO LATTICE DYNAMICS USING REVERSE MONTE CARLO AND FORCE FIELD METHODS

Julija Lukasevica, Andris Anspoks, Aleksandr Kalinko, Alexei Kuzmin

Institute of Solid State Physics, University of Latvia

Keywords
NiO, lattice dynamics, EXAFS, reverse Monte Carlo, force field method

Actuality and aim

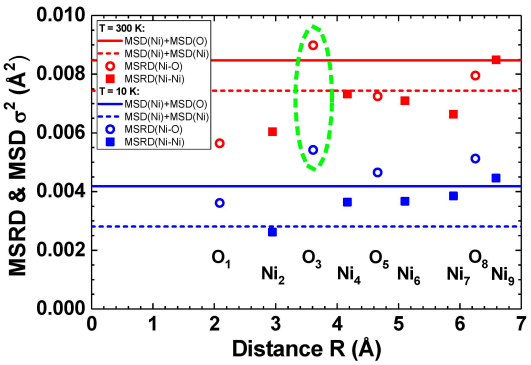
The lattice dynamics of the Mott-Hubbard insulator NiO with a magnetic Néel phase transition at 523 K has been the subject of numerous studies for many years. However, until now, the accent of most investigations has been paid to phonon frequencies [1]. In this study, we discuss the temperature dependence of the amplitudes of thermal vibrations in NiO obtained from the extended X-ray absorption fine structure (EXAFS) spectra.

Methods

Mean-square relative displacements (MSRD) for Ni-O and Ni-Ni atom pairs were determined from the Ni K-edge EXAFS spectra using two methods: (i) reverse Monte Carlo (RMC) simulation [2] and (ii) lattice dynamics with the force field model from [3]. The chosen force field model was validated by comparing the experimental EXAFS spectrum with the results of molecular dynamics simulations.

Results

MSRD factors were obtained for the nearest nine coordination shells of nickel in the temperature range of 10-300 K. Their values for distant shells approach, as expected, the sum of the mean-square displacements of Ni and Ni/O atoms, taken from [4]. We found that the values of the MSRD factor for the Ni-O_3 atom pair (involving O atoms in the 3rd coordination shell of nickel) obtained by the RMC method are unexpectedly large at all temperatures.



MSRD and MSD 2 factors for the first nine coordination shells around nickel atoms in NiO at T=10 an

Conclusions

The observed results can be explained by the fact that the correlation of atomic motion between the Ni and O_3 atoms located along with the <111> crystallographic directions is significantly reduced due to weak interatomic interaction.

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EXAFS STUDY OF LATTICE DYNAMICS IN METALS WITH CUBIC AND HEXAGONAL STRUCTURES USING THE REVERSE MONTE CARLO METHOD

Vitalijs Dimitrijevs, Alexei Kuzmin

EXAFS spectroscopy laboratory, Institute of Solid State Physics, University of Latvia

Keywords
Zn, Cd, Mo, EXAFS, lattice dynamics, reverse Monte Carlo method

Actuality and aim
Atomistic simulations based on empirical potentials are widely used to study pure metals and their alloys. However, such models have difficulty reproducing the structure and dynamics of hexagonal close-packed (hcp) compounds as, for example, Zn [1] and Cd [2]. In this study, we use the extended X-ray absorption fine structure (EXAFS) spectroscopy to probe the local lattice dynamics in hcp Zn and Cd in comparison with the body-centered cubic (bcc) Mo.

Methods
The metal (Mo, Cd, Zn) K-edge EXAFS spectra were analysed using the reverse Monte Carlo (RMC) method [3] taking into account the multiple-scattering effects. Classical molecular dynamics (MD) simulations were additionally performed for bcc Mo and hcp Zn at 300 K for comparison. The MD results were validated using the EXAFS spectra measured at 300 K.

Results
The structural models obtained from the RMC simulations reproduce well the experimental EXAFS spectra for all studied metals. As expected, the MD simulation of bcc Mo is in good agreement with the EXAFS data, while for hcp Zn, a significant disagreement was found. Mean-square relative displacements (MSRDs) for Mo-Mo, Cd-Cd and Zn-Zn atom pairs were determined from the radial distribution functions obtained by RMC and MD simulations.

Conclusions
RMC method allows one to extract information on MSRD factors for distant coordination shells from the analysis of EXAFS spectra. This opens up the possibility of estimating the MSRDs as well as the mean-square displacements of atoms from a single experiment, as the correlation in atomic motion becomes negligible for distant atoms.

Acknowledgements
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DIRECT OBSERVATION OF CRYSTAL FIELD SPLITTING IN TUNGSTATES BY RESONANT X-RAY EMISSION SPECTROSCOPY

Alexei Kuzmin [1], Aleksandr Kalinko [2], Inga Pudza [3], Georgijs Bakradze [3], Maria A. Naumova [2]

[1.] Institute of Solid State Physics, University of Latvia, Kengaraga street 8, LV-1063 Riga, Latvia , [2.] Deutsches Elektronen-Synchrotron (DESY) – A Research Centre of the Helmholtz Association, Notkestrasse 85, D-22607 Hamburg, Germany, [3.] Institute of Solid State Physics, University of Latvia, Kengaraga street 8, LV-1063 Riga, Latvia

Keywords
Resonant X-ray emission spectroscopy, Crystal-field splitting

Actuality and aim

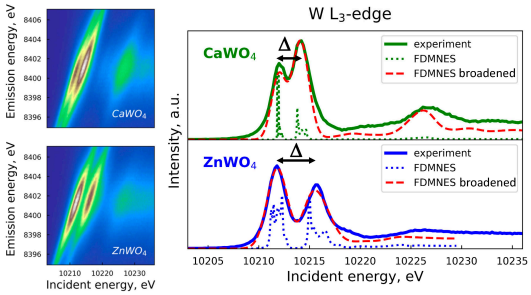
Resonant X-ray emission spectroscopy (RXES) is a photon-in photon-out X-ray technique providing information on the electronic states of metal with element selectivity and high energy resolution. It was successfully employed by us recently to study phase transitions in $CuMo_{1-x}W_xO_4$ solid solutions [1]. Here we demonstrate the sensitivity of the method to crystal field splitting in a series of AWO_4 (A=Mg, Ca, Zn, Cd, Sn, Pb) tungstates.

Methods

Polycrystalline tungstates were studied using the RXES technique by detecting W L_beta1 and L_alfa1 emission while scanning across the W L2,3-edges. The RXES map measurements were performed using von Hamos-type X-ray emission spectrometer at the HASYLAB DESY PETRA-III beamline P64 [2,3], and high-energy resolution fluorescence detected X-ray absorption near-edge structures (HERFD-XANES) were determined from the RXES maps. They were interpreted using the full-multiple-scattering XANES calculations using ab initio real-space FDMNES code [4].

Results

The RXES maps and corresponding HERFD-XANES spectra (see figure for Ca(Zn)WO4) reveal the structure of the unoccupied W 5d states and their splitting in the tetrahedral (1.3-2.0 eV) and octahedral (3.6-3.9 eV) crystal fields. The experimental results agree well with the calculations.



Experimental RXES maps and HERFD-XANES spectra for $CaWO_4$ and ZnWO4 compared with the calculations.

Conclusions

Thus, RXES allows one to probe the splitting of the conduction band states in tungstates. The type of the splitting can be used as a fingerprint for different crystal lattices.

Acknowledgements

Financial support by the Latvian Council of Science project no. lzp-2019/1-0071 is acknowledged.

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INERT COATINGS FOR CYCLE LIFE EXTENSION OF CATHODES FOR LI-ION BATTERIES

Liga Britala [1], Maris Knite [2], Gints Kucinskis [1]

[1.] Institute of Solid State Physics, University of Latvia, [2.] Riga Technical University, Latvia

Keywords
Li-ion batteries, cathode, NCM111, coating, wet-chemical

Actuality and aim

During the operation of Li-ion batteries, a cathode-electrolyte interface is formed on the cathode material within the battery cells which increases the internal resistance and traps lithium into various compounds [1]. Additionally, the mechanical integrity of the cathode material is disrupted by continuous intercalation and deintercalation of lithium ions [2]. One of the solutions to prevent these undesired changes is to synthesize a chemically and thermodynamically inert coating on the surface of the cathode material [3].
The aim of this work is to develop a wet-chemical method to obtain a uniform Al_2O_3 coating on NMC111 cathode material for cycle life extension.

Methods

$Al(OC_3H_7)_3$ or $Al(NO_3)_3$ was utilized as the aluminium raw material. The coating was synthesized via a wet-chemical method followed by calcination at 500°C to obtain the Al_2O_3-coated cathode material.
The coated material was analysed using XRD and SEM methods. To test the effect of the coating on battery cycle life, battery cells were assembled and galvanostatic charge-discharge measurements were performed.

Results

It was observed that despite a slight reduction in rate capability, after 500 full charge-discharge cycles the Al_2O_3-coated material showed higher specific capacity and thus – longer lifespan. No change in crystal structure and morphology of the cathode particles was observed for the coated samples.

Conclusions

Al2O3 coating increases the stability and improves the electrochemical performance of NMC111 cathode material.

Acknowledgements

The financial support of ISSP UL Student and Young Scientists project 2021/2022 is greatly acknowledged.

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ON THE EFFICIENCY OF HYDROGEN PRODUCTION FROM PLASMA-TREATED ALUMINUM WASTE WITH NAOH AND KOH PROMOTERS

Ansis Mezulis [1], Peteris Lesnicenoks [1], Ainars Knoks [1], Marius Urbonavicius [2], Sarunas Varnagiris [2]

[1.] Institute of Solid State Physics of University of Latvia, [2.] Center for Hydrogen Energy Technologies, Lithuania

Keywords
waste aluminum, hydrogen generation, hydrogen plasma treatment

Actuality and aim
New methods to generate energy is an actual issue due to concerns about the depletion of fuels. Hydrogen is a promising source of energy because it affords a clean and high heat of combustion. There are several advantages of using aluminum as a primary source of hydrogen production, especially, if aluminum is utilized from recyclable materials, such as dross and soft drink cans. Although the reaction between aluminum and water at the ambient temperature is thermodynamically favorable, it is hindranced by coherent and adherent layers of aluminum oxide on the surface of aluminum particles. The aim of this work is, besides using an alkali promoter to disrupt the oxide layer, to apply an effective aluminum particles pre-treatment [1].

Methods
Aluminum particles are pre-treated by means of acting with low-temperature hydrogen gas plasma. It changes nano-scale topography of the surface and creates polar groups. After the pre-treatment the reaction is running in a standard reactor. Alkali, NaOH or KOH, is not consumed in the reaction and acts as a catalyst.

Results
The activation energy Ea is evaluated from experiments at different temperatures. Approximated values of Ea is slighty dependent on chosen alkali. Our plasma-treated aluminum sample in reaction with 0.5M NaOH reached Ea=56.4 kJ/mol. It is 18% less than reported 68.5 kJ/mol in Ref. [2], being a considerable advantage for the chemical reaction to occur. Second, the reaction rate is calculated for all performed experiments, being ca. 2 times higher with plasma-treated aluminum samples.

Conclusions
Applied plasma-treatment to aluminum particles proves to decrease the activation energy and to increase the reaction rate.

Acknowledgements
Baltic Research Programme No. EEA-RESEARCH-92, EEA Grant No. EEZ/BPP/VIAA/2021/5

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CHARACTERIZATION OF OXIDES IN THE PRVOX-CAVOX SYSTEM FOR SOLID OXIDE FUEL CELL APPLICATIONS

Rui Pinto, Blanca Arias-Serrano, Aleksey Yaremchenko

CICECO - Aveiro Institute of Materials, University of Aveiro, Portugal

Keywords
fuel cell, vanadate, electrical conductivity, redox stability

Actuality and aim
Rare-earth and alkaline-earth vanadates attract attention as redox-reversible components for fuel electrodes of solid oxide fuel cells (SOFC). An advantage of (Ln,A)VO_x-derived components is their anticipated resistance to carbon deposition and sulfur-containing impurities, which is critical for hydrocarbon- and biogas-fueled SOFCs. The present work was focused on the oxides of the $PrVO_4$-$Ca_2V_2O_7$ system as fuel electrode precursors, with an emphasis on phase relationships, redox behavior, thermomechanical and electrical properties.

Methods
$Pr_{1-x}Ca_xVO_{4-\delta}$ (x = 0-0.20) and $Ca_2V_2O_7$ were prepared by the solid-state route. Ceramics samples were sintered in air at 1000°C for $Ca_2V_2O_7$ and 1300°C for other materials.

Results
XRD demonstrated the formation of phase-pure $Pr_{1-x}Ca_xVO_{4-\delta}$ solid solutions with the tetragonal zircon-type structure for up to 5 at.% of Ca in Pr sublattice. At the same time, SEM/EDS suggest a lower solubility indicated by the presence of Ca-V-O phase impurities. Doping by calcium increases mixed ionic-electronic conductivity of Pr(Ca)VO_4 ceramics under oxidizing conditions. The electronic contribution is p-type and decreases with reducing $p(O_2)$. The reduction of Pr1-xCaxV04-δ ceramics in a 10%H_2-N_2 atmosphere at 800°C leads to phase separation and formation of perovskite-like $PrVO_3$ and $CaVO_3$ phases. The redox behavior of $PrVO_4$-$Ca_2V_2O_7$ ceramics on isothermal cycling between air and 10%H_2-N_2 was studied by impedance spectroscopy, thermogravimetry, dilatometry and post-mortem XRD analysis.

Acknowledgements
This work was supported by the FCT/MCTES/FEDER (projects CARBOSTEAM (POCI-01-0145-FEDER-032295) and CICECO-Aveiro Institute of Materials (UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020), and PhD grant 2020.04654.BD).

ANALYSIS OF LITHIUM IRON PHOSPHATE SERVICE LIFE IN LI-ION BATTERIES AT DIFFERENT TEMPERATURES AND CYCLING RATES

Julija Hodakovska, Gunars Bajars, Gints Kucinskis

Institute of Solid State Physics, University of Latvia

Keywords
Li-ion battery; lithium iron phosphate; electrode ageing; service life

Actuality and aim
Lithium ion batteries (LIBs) are widely used in different areas: portable devices, transport and stationary energy storage; each having different demands. This rises multiple challenges, e.g., search for materials that would either prolong the service life of LIBs or would use more abundant compounds like sodium. Apart from the global goals, some issues need to be addressed on the level of ordinary users. Recent supply chain issues increased the need to predict the moment when the LIB should be changed, enabling a timely order of the replacement part. Our ongoing project characterizes the electrochemical behavior of lithium iron phosphate (LFP) cathode for LIBs at different service life stages to enable prediction of the electrode ageing.

Methods
LFP half-cells are deep-cycled at different rates and temperatures. To further understand the underlying ageing processes, impedance spectroscopy, as well as structural and morphological characterization are used.

Results
Dependencies related to ageing are determined and related to corresponding processes for LFP cathode in a half-cell. The analysis of overvoltage during charging and discharging processes shows promising results for the estimation of the state of health without implementing complex measurements.

Conclusions
Acquired results and previous experience in testing of commercial cells [1] will be further used in modeling behavior of full-cells to build model that is capable to estimate state of health and/or predict remaining service life.

Acknowledgements
The financial support of LZP-2020/1-0425 project “Cycle life prediction of lithium-ion battery electrodes and cells, utilizing current-voltage response measurements” is greatly acknowledged.

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AMPHOTERIC DECOUPLED WATER ELECTROLYSIS FOR HYDROGEN PRODUCTION

Martins Vanags, Andris Šutka

Riga Technical University, Latvia

Keywords
decoupled electrolysis, amphoteric

Actuality and aim

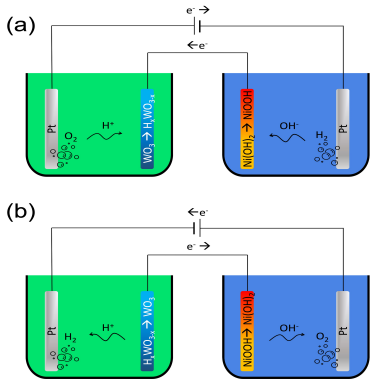
Here we show the concept for amphoteric decoupled electrolysis [1]. Water electrolysis takes place in two separate cells, one of which is filled with an alkaline electrolyte and the other with an acid electrolyte. OER and HER reactions take place alternately in separate cells. This concept allows to obtain extremely high efficiency in one of the reaction directions.

Methods

The cell of the proposed electrolysis are shown in Figure. Two primary Pt electrodes were placed in separate cells - cathode in acid cell and anode in the alkaline cell for realizing HER or OER. The WO_3 and $Ni(OH)_2$ were used as auxiliary electrode materials to provide operation in acidic and basic media, respectively.

Results

At the first cycle (unfavourable), during the water splitting, the tungsten oxide is protonated to tungsten bronze and nickel hydroxide is transformed to nickel oxyhydroxide. In the other cycle (favourable) situation is opposite.



Decoupled amphoteric electrolysis operating in two different modes.

Conclusions

The potential for gas generation depends on the polarity of the applied potential. In the first cycle, simultaneous water splitting and ion accumulation in AEs occur. In the second cycle, hydrogen and oxygen are generated in acid and alkaline cells, respectively, from ions released from AEs. The total energy efficiency of the provided electrolysis concept is up to 71%.

Acknowledgements

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1. DOI: 10.1039/D1EE03982B

LEACHING OF VALUABLE METALS FROM SCRAP PRINTED CIRCUIT BOARDS UNDER THE ACTION OF ALTERNATING CURRENT

Vera Serga [1], Maksims Kuzmins [1], Aleksej Zarkov [2], Edgars Elsts [2], Vladimir Pankratov [2]

[1.] Institute of Materials and Surface Engineering, Faculty of Materials Science and Applied Chemistry, Riga Technical University, P. Valdena 7, LV-1048 Riga, Latvia, [2.] Institute of Solid State Physics, University of Latvia, Kengaraga 8, LV-1063 Riga, Latvia

Keywords
Alternating current, printed circuit boards, gold, copper, leaching, chlorine

Actuality and aim
Recycling of secondary raw materials is an important aspect of the sustainable development of modern industry and energetics. This work is aimed at studying the leaching process of Au and Cu from computer printed circuit boards (PCBs) under the action of industrial frequency AC in hydrochloric acid solutions.

Methods
PCBs were crushed by a disintegrator [1] and separated into three fractions: 1 - <0.09 mm, 2 - 0.18-0.09 mm and 3 - 0.35-0.18 mm. The phase and elemental composition of solid materials was studied by X-ray diffraction (XRD) and X-ray fluorescence (XRF) methods. Quantitative analysis of metals in solutions was carried out by inductively coupled plasma – optical emission spectrometry (ICP-OES).

Results
The results of ICP-OES showed that the content of metals in the raw material depends on the fractional size of the particles. So fraction 1 contains the highest amount of Au (0.08%) and the lowest content of Cu (1.40%), whereas, fraction 3 contains only 0.01% of Au, but 6.13% of Cu. It was found that under the same experimental conditions, namely, i = 0.66 A/cm2, t = 2h, solid-liquid ratio - 8.6 g/l, complete leaching of gold from PCBs fractions 2 and 3 is achieved when the degree of Cu leaching is 84.6% and 95.2%, respectively.

Conclusions
The research results showed the possibility of successful combination of two processes - the generation of an oxidizing agent (chlorine) and the leaching of metals from PCBs scrap in one electrolytic cell using the alternating current.

Acknowledgements
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REACTOR DESIGN INVESTIGATION FOR HYDROGEN PRODUCTION FROM ALUMINIUM -WATER REACTION

Raitis Kaspars Sika, Pēteris Lesničenoks, Jānis Kleperis, Vladimirs Ņemcevs, Jūlija Hodakovska, Roberts Oliņš, Ainārs Knoks

Institute of Solid State Physics, University of Latvia and Faculty of Applied Chemistry and Material Sciences

Keywords
Hydrogen energetics, recycling, cyclic economy, aluminium

Actuality and aim
Aluminium is one of vastly landfilled materials despite the potential for recycling. One prominent use is hydrogen production through reaction with water [1]. The aim of the study is to compare new reactor design influence on hydrogen production and particle behaviour via SolidWorks Flow simulation comparison to empirical reactor that is compared to conventional and stationary reactor [2].

Methods
A model of the reactor recreated in SolidWorks software and analyzed with SolidWorks Flow Simulation. Gained model is compared to reactor prototype for comparison. Finally, reactor design is compared to conventional stationary reactor.

Results
Built design was modeled with SolidWorks Flow simulation to compare particle behaviour and its influence on the production of hydrogen. Comparison of new design with conventional reactor was carried out.

Conclusions
Based on the gained results flow simulation can provide adequate addition to geometry investigation and new reactor design even with gas production particles and changes in electrolyte composition i.e. AL dissociation and production of oxides and hydroxides.

Acknowledgements
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PROPERTIES OF "MICROCRYSTALLINE CELLULOSE - $KBI_{1-X}PR_X(MOO_4)_2$" NANOCOMPOSITES

Serhii Nedilko [1], Vasyl Scherbatskii [1], Kateryna Terebilenko [1], Andrzej Suchocki [2], Zhydachevskyy Yaroslaw [2], Vytalii Chornii [3], Vadym Sheludko [4], Olga Gomeniyuk [5]

[1.] Taras Shevchenko National University of Kyiv, Ukraine, [2.] Institute of Physics Polish Academy of Science, Poland, [3.] National University of Life and Environmental Sciences of Ukraine, [4.] Oleksandr Dovzhenko Hlukhiv National Pedagogical University, Ukraine, [5.] , Ya. Zhydachevskyy2), V. Chornii1,3) V. Sheludko4), O.

Keywords
phosphor, RE ions, covers, cellulose

Actuality and aim
In the most of commercial WLEDs the InGaN semiconductor chip is covered by phosphor that allows modifying of LEDs emission spectrum. Now, attention is paid to phosphor which have intensive PL in the red spectral range and oxide compounds doped with RE ions (Eu^{3+}, Pr^{3+}, Sm^{3+}, etc.) belong to them. At the same time, polymers, e.g. silicones, play a role of host for noted micro- or nano-crystalline phosphors. Cellulose is eco-friendly natural polymer, that is why, it is an alternative for the polymer host

Methods
The procedure of the samples preparation, morphology and luminescence properties of composites those consist of cellulose matrix and praseodymium-doped potassium bismuth molybdate micro- and nanoparticles as filler are reported here

Results
Microscopy had shown the homogeneity of the samples in the scale above 100 .m The sizes of oxide particles were in the range from ~ 100 nm up to 3 nm The samples revealed intensive PL both of Pr^{3+} ions and micro-cellulose.
The study of influence of temperature on luminescence characteristics of composites in the temperature range 18 – 75 °C showed that intensity of Pr^{3+} - related luminescence decreases on about 40 % while cellulose-related photoluminescence decrease on about 20%.

Conclusions
Thus, studied composites are prospective materials for elaboration of luminescent covers for low power WLEDs.

Acknowledgements
Acknowledgement. This work was partially financed by Ministry of Education and Science of Ukraine and supported by Institute of Physics PAN, Warsaw.

ELECTROCHEMICAL CORROSION BEHAVIOR OF ALUMINUM FOIL – INVESTIGATION OF KITCHEN WASTES

Ainars Knoks [1], Janis Kleperis [1], Peteris Lesnicenoks [1], Ansis Mezulis [1], Julija Hodakovska [1], Raitis Sika [1], Marius URBONAVICIUS [2], Sarunas VARNAGIRIS [2], Camila Pia Canales Oyarzo [3], Christiaan Richter [3]

[1.] Institute of Solid State physics, University of Latvia, [2.] Center for Hydrogen Energy Technologies, Lithuanian Energy Institute, [3.] UNIVERSITY OF ICELAND

Keywords
aluminium, hydrogen energetics, recycling, electrochemistry

Actuality and aim
Aluminium is entering waste bins. Waste Al can react with both acidic and caustic electrolytes. Research on the use of Al in hydrogen energetics has become more prominent as the circular economy develops. There is a lack of knowledge of the reaction process. The goal of the study is to investigate waste Al-H_2O reaction.

Methods
Al-H_2O reaction for hydrogen production is fundamentally a corrosion reaction. When Al is immersed in an aqueous environment, oxidation and reduction reactions occur until an equilibrium. The corrosion potential and current can be altered by the environment. Investigation was carried out via electrochemical corrosion measurements. Measurements were carried out in NaOH, KOH, KCl, NaCl and deionized water at various temperatures.

Results
Electrolyte has great influence on the chemical potential at which hydrogen is produced as well as reaction mechanism. Temperature shifts the corrosion potential to more positive values.

Conclusions
Investigation of Al-H2O gives insights into reaction kinetics. Identification of correct electrolyte and reaction parameters determines the scalability and costs of large scale hydrogen production via AL-water reaction

Acknowledgements
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APPLICATION OF THE DISINTEGRATION GRINDING METHOD TO INCREASE THE EFFICIENCY OF THE PROCESSING OF USED PRINTED CIRCUIT B

Ervīns Blumbergs, Andrejs Šiškins

Limited Liability Company Scientific and Technical Company "AERKOM", Latvia

Keywords
Extraction of valuable metals, Pretreatment of printed circuit boards

Actuality and aim
Pretreatment of printed circuit boards before the extraction of valuable metals.

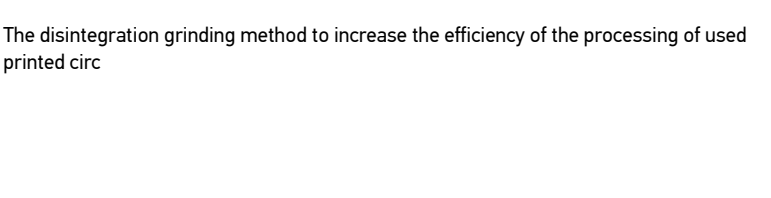
Methods
The disintegration method is based on the high-energy impact of the particles of the material to be ground, thus causing the separation of the metallic components of the printed circuit boards.

Results
In the course of the work, single and double direct grinding by the method of disintegration was studied. the bulk density of various fractions of the crushed material was studied and the bulk density was correlated with the metal content in this fraction

Application of the disintegration grinding method to increase the efficiency of the processing of used printed circuit boards.

Authors: E. Blumbergs, A.Shishkin

The paper considers the method of pretreatment of printed circuit boards before the extraction of valuable metals. The disintegration method is based on the high-energy impact of the particles of the material to be ground, thus causing the separation of the metallic components of the printed circuit boards. In the course of the work, single and double direct grinding by the method of disintegration was studied. the bulk density of various fractions of the crushed material was studied and the bulk density was correlated with the metal content in this fraction



Conclusions
This method allows you to prepare electronic boards for the extraction of valuable metals by the electrochemical method.

Acknowledgements
The work was supported by project nr.1.1.1.1/20/A/139

References
Preparation of electronic boards for the extraction of valuable metals.

HALLOYSITE/POLYANILINE NANOCOMPOSITES FOR REMOVAL OF DYES AND DICHROMATE POTASSIUM FROM WATER

Yuriy Noskov [1], Valery Bliznyuk [2], Alexander Pud [1]

[1.] V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of the National Academy of Sciences of Ukraine, 50 Kharkivske Shose, 02160 Kyiv, Ukraine, [2.] Environmental Engineering & Earth Sciences, Clemson University, Clemson, SC 29634, USA

Keywords
Halloysite/polyaniline, dopant, nanocomposites, removal, toxic substances

Actuality and aim
Decontamination of natural waters from industrial pollutants is an important environmental issue. Our research is focused on development of new biocompatible nanocomposites based on halloysite nanotubes (HNT) with high sorption ability [1] and polyaniline (PANI) doped with natural multifunctional phytic acid (PA) [2] suitable for effective absorption of the pollutants from aqueous media.

Methods
TEM, FTIR and UV-Vis-spectroscopy, thermogravimetry (TGA), conductivity and adsorption measurements

Results
Synthesized core-shell nanocomposites have tubular architecture with high surface area due HNT core and possess electrical conductivity due to the presence of doped PANI-PA shells. TGA and spectroscopy revealed strong interaction between the components, which affect thermostability, conductivity and adsorption behavior of the nanocomposites also leading to their non-linear dependence on the PANI-PA content. We demonstrate as an example the removal of organic dyes (methylene blue, methyl orange) and dichromate potassium from contaminated water with UV-Vis-spectroscopy monitoring of the process. The sorption capacity depends on the PANI-PA loading and the type of adsorbate (charge, functional groups, redox-potential). The sorption kinetics is described by pseudo-second order model in all cases.

Conclusions
Novel biocompatible hybrid HNT/PANI-PA nanocomposites have been synthesized for efficient removal of different toxic pollutants from water. Their effectiveness as the sorbents depends on the PANI-PA content in the nanocomposite and the nature of the pollutant.

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STEALTHY MAGNETIC LIPOSOMES FOR DRUG DELIVERY

Mart Ernits [1], Olavi Reinsalu [2], Immanuel Sanka [3], Reet Kurg [2], Andreas Kyritsakis [2], Veronika Zadin [2]

[1.] PhD student at the University of Tartu, Estonia, [2.] University of Tartu, Estonia, [3.] Tallinn University of Technology, Estonia

Keywords
Magnetic liposomes, microfluidics

Actuality and aim
Magnetic liposomes are a promising method for localised drug delivery in cancer treatment. Contrary to the current state-of-the-art where magnetic particles are attached to the liposome's outer surface, this work aims to develop magnetic liposomes with magnetic particles attached to the inner membrane. Thus reducing the exposure of tissues to foreign elements and unnecessary immune system activation.

Methods
Solvent inversion techniques as well as a microfluidics based approach, are used to produce liposomes with the magnetic nanoparticles attached to the inner membrane. Mineral oils and octanol are tested as oil-phase solvents for phospholipid formation. Optical microscopy is used for in-situ inspection of the liposome formation, enabling real life control for process optimisation. Pictures of the microfluidic chips and some results will be included.

Results
Two different approaches of liposome production, i.e. solvent inversion and microfluidics, are evaluated for their yield and time-effectiveness. The best overall technique along with the configuration of input materials is proposed as the next step for a PhD research project about remotely localised drug delivery for cancer treatment.

Conclusions
Solvent inversion is too unreliable for this application.

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AMORPHOUS CALCIUM PHOSPHATE SUSPENSIONS AS A WAY TO ATTAIN BIOACTIVITY OF PEO COATINGS

Vladlens Grebņevs [1], Yevheniia Husak [2], Şahin Altundal [3], Aleksandrs Dutovs [4], Katarzyna Leśniak-Ziółkowska [5], Marta Wala [5], Roman Viter [3], Arturs Vīksna [6], Wojciech Simka [5]

[1.] University of Latvia, Faculty of Chemistry (Riga, Latvia); Silesian University of Technology, Faculty of Chemistry (Gliwice, Poland), [2.] Sumy State University, Biomedical Research Center (Sumy, Ukraine); Silesian University of Technology, Faculty of Chemistry (Gliwice, Poland), [3.] University of Latvia, Institute of Atomic Physics and Spectroscopy (Riga, Latvia), [4.] University of Latvia, Institute of Chemical Physics (Riga, Latvia), [5.] Silesian University of Technology, Faculty of Chemistry (Gliwice, Poland), [6.] University of Latvia, Faculty of Chemistry (Riga, Latvia)

Keywords
plasma electrolytic oxidation, crystallinity, bioactivity, hydroxyapatites

Actuality and aim
One way to improve characteristics of oxide coatings prepared by plasma electrolytic oxidation (PEO) method in suspensions lies in variation of solid particle properties [1]. To date, particle size, phase composition and thermal stability are known to have considerable impact. In this study, the effect of particle crystallinity on physicochemical properties and bioactivity of coatings prepared on Ti and Ti6Al4V substrates was studied.

Methods
PEO was performed in DC mode at 350 V in electrolytes containing 100 g/L of crystalline hydroxyapatite or amorphous tricalcium phosphate (TCP) particles with average size of ~450 nm. Series of measured parameters included oxide layer thickness, surface wettability, roughness, topography, as well as cross-sectional chemical composition. Simulated body fluid tests were applied to assess coating bioactivity.

Results
Particle crystallinity had a tangible specific effect on apatite layer growth dynamics during SBF tests and topography, which was reflected in the modification of the pore shape, average size and total surface porosity. Influence of particle crystallinity on those incorporation pattern showed high repeatability depending on the elemental composition of the investigated substrates.

Conclusions
Based on the regularities discovered, utilization of amorphous TCP particles as a PEO electrolyte additive can be proposed as preferable for implantology issues to obtain oxide coatings with increased micro-roughness, wettability and calcium phosphate content. Ultimately, combination of these characteristics ultimately promotes higher bioactivity of the PEO coating surface.

Acknowledgements
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TIME-RESOLVED FLUORESCENCE TO DETERMINE THE VIABILITY OF BACTERIAL SPORES

Ott Rebane, Marco Kirm, Juhan Saaring, Vitali Nagirnyi

University of Tartu, Estonia

Keywords
Time-resolved fluorescence; bacterial spores; decontamination; H_2O_2 vapor

Actuality and aim

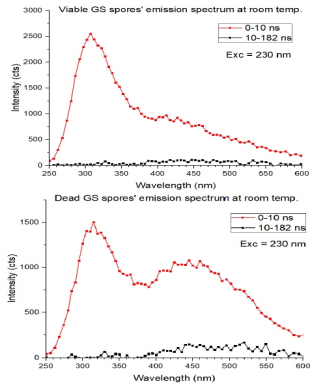
As risks posed by multidrug-resistant bacteria as well as other pathogens are constantly relevant in modern society, monitoring the efficiency of the decontamination of rooms and surfaces cannot be overstated [1]. In this study we look at the possibilities to estimate the efficiency of vaporised hydrogen peroxide procedures by distinguish between the time-resolved spectra of bacterial spores killed by vaporised hydrogen peroxide and the spores that are still viable.

Methods

Vaporised hydrogen peroxide (VHP) at ~600 ppm is used to decontaminate Geobacillus stearothermophilus bacterial spores on stainless steel surface. Viable spores that have not been treated by VHP are measured as a comparison. The time-resolved fluorescence of the samples is studied in the UVC excitation regions with the P66 beamline. The excitation, emission and time-resolved spectra of dead and viable spores are compared.

Results

Distinct differences between the dead and viable spores are present in various measurement modes. The emission spectra show a stark decrease in the amino-acid-fluorescence spectral region for the dead spores, while the time-resolved spectra show shortening of the relevant decay time in the same region. The spectral region connected to oxidation results shows different behaviour.



Comparison of the emission spectra of VHP-treated and viable bacterial spores, when excited at 230nm

Conclusions

Although viable and dead spores do have differences in the time-resolved spectra, these are small enough so that the development of a small hand-held sensor based on these results is not considered a good investment yet.

Acknowledgements

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