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INSTITUTE OF SOLID STATE PHYSICS UNIVERSITY OF LATVIA





FUNCTIONAL MATERIALS & NANOTECHNOLOGIES

12th International Scientific Conference on Functional Materials and Nanotechnologies

FM&NT-2018

October 2- 5, 2018, Riga, Latvia

PROGRAM

WELCOME MESSAGE TO FM&NT-2018 PARTICIPANTS

DEAR COLLEAGUES,

It is my great pleasure to welcome you at the 12th International Conference Functional Materials and Nanotechnologies (FM&NT), and to Riga.

In 2018, Latvia celebrates a hundred years since it became an independent state. Our neighbours - Estonia and Lithuania – are celebrating their centenaries of statehood as well. With festivities at home and all around the world, the Baltic countries will present the best they can offer in culture, lifestyle, and innovation. The arranged FM&NT-2018 conference on advanced materials and nanotechnologies falls under materials scientist's contribution in this year of the Baltic countries national anniversaries.

This conference is a continuation of annual meetings, first of which was organized in 2006 by the Institute of Solid State Physics, University of Latvia (ISSP UL) in Riga. Since 2013 FM&NT conferences turned over a new page – becoming a common conference of all three Baltic countries. Now it is being organized periodical by the ISSP of University of Latvia, University of Tartu, and Vilnius University. FM&NT is also a tribute to 40ty year jubilee of the ISSP UL and Centenary celebration of the University of Latvia in 2019. The purpose of the conference is to bring together materials scientists, physicists, chemists, research staff, engineers, as well as experts in a wide range of the most demanding application areas, and 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 yet more. 6 plenary talks, 19 invited talks, 37 oral presentations and over 130 posters of high scientific quality will be given at the conference. The joint event will also provide a platform for the future collaboration promoting interdisciplinary research.

The FM&NT-2018 conference will take place in Radisson Blu Latvia Conference & Spa Hotel in Riga. The Conference dinner and excursion will be held in Riga Motor Museum. The museum showcases more than a hundred unique antique vehicles and the collection is enriched with several significant acquisitions. Exploration the world of vehicles and their history of development could have some added scientific value for participants, e.g. to rouse new ideas on development of automotive batteries or other accessories, sensors and actuators for diagnostics and for realizing artificial intelligence prospects.

I wish to thank International Organizing and Program Committees, as well as Local Committees members for hard working preparing the Conference.

Thank you all for coming and I wish you most successful and pleasurable conference!

Andris Sternberg, Chairman of FM&NT-2018 Institute of Solid State Physics, University of Latvia, Riga, Latvia

SCIENTIFIC TOPICS OF THE FM&NT-2018

THEORY:

Theory and computational material science by atomistic scale modelling of technologically important materials and devices

FUNCTIONAL MATERIALS:

Functional (inorganic, organic and hybrid) materials for electronics and photonics

NANO:

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

ENERGY:

Perspective materials and technologies for harvesting and storage of renewable energy: hydrogen, fuel cells, photovoltaics, piezoelectric, thermoelectric, LED and OLEDs, and developing of diverse energy systems.

LIST OF PREVIOUS FM&NT CONFERENCES

Riga (Latvia)	2006
Riga (Latvia)	2007
Riga (Latvia)	2008
Riga (Latvia)	2009
Riga (Latvia)	2010
Riga (Latvia)	2011
Riga (Latvia)	2012
Tartu (Estonia)	2013
Riga (Latvia)	2014
Vilnius (Lithuania)	2015
Tartu (Estonia)	2017

Joint RCBJSF and FM&NT Symposium

FM&NT-2018 COMMITTEES

Conference Chairman: Dr.habil. Andris Sternberg

FM&NT INTERNATIONAL ORGANIZING COMMITTEE

- Prof. Jūras Banys, Lithuania
- Prof. Antonio Bianconi, Italy
- Prof. emeritus Niels Egede Christensen, Denmark
- Prof. Robert Evarestov, Russia
- Prof. Claes-Göran Granqvist, Sweden
- Prof. Marco Kirm, Estonia
- Dr. Jiri Kulda, France
- Prof. Ergo Nõmmiste, Estonia
- Dr. Toomas Plank, Estonia
- Dr. Martins Rutkis, Latvia

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- Dr. Andris Sternberg
- Dr. Qin Wang

Anatolijs Šarakovskis, Jurģis Grūbe, Elīna Pavlovska, Līga Klēbaha, Anna Grūbe, Inga Jonāne, Ivita Bite, Arturs Cintiņš, Ingars Lukoševičs, Inese Takere, Raitis Siatkovskis

Committees sincerely hope that the FM&NT-2018 conference will give all the participants new insights into the wide spread development of functional materials and nanotechnologies, will enhance the circulation of information released at the meeting, and will bring new friends, contacts and common projects! **Thank you all for coming and we wish you successful and enjoyable conference.**

USEFUL CONTACT PHONES

Conference chairman: Dr.habil.phys. Andris Sternberg (mobile)	+371 26183061
Local committee chairlady: Liga Grinberga (mobile)	+371 26415673
Hotel:	
Radisson Blu Latvia Conference & Spa Hotel	+371 67772222





PUBLISHERS OF THE CONFERENCE PAPERS:



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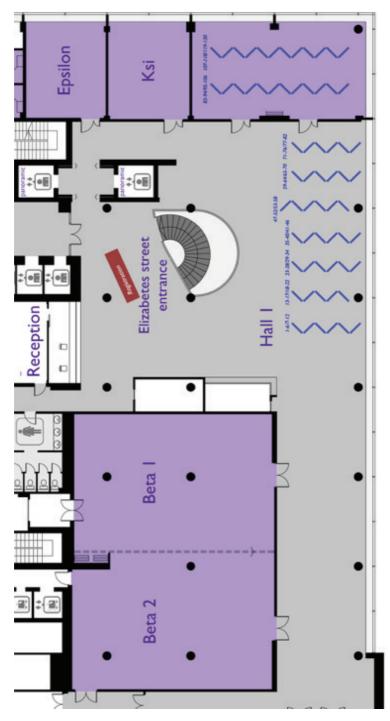
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FM&NT-2018 SITE



FM&NT-2018 AGENDA AT A GLANCE

October 2		Octo	October 3			Ocother 4	er 4			Octo	October 5	
16:00 Registration	8:30	Re	Registration	u	8:30	Re	Registration	u	8:30	R	Registration	u
17:00 Webene	X	E	Beta Hall		X	B	Beta Hall		9:00	Coffe	Coffee 9:00 - 9:30	9:30
18:30 wexcuie party	8:50	Techino	Techincal information	nation	9:00	Techincal information	al infor	nation	X	Beta hall 1	X	Beta hall 2
		Opening - Conference chairman A.Sternberg, D.	nce chairm	an A.Sternberg, D.	9:10	Andı	Andrei Kholkin	kin	9:30	<u>J. Pflaum</u>	9:30	<u>A. Lipovski</u>
	00-0	Stepanovs (Ministry of Education and Science), V.	of Educati	on and Science), V.	10:10	Aharo	Aharon Gedanken	nken	10:00	L. Vieira	10:00	M. Chou
Plenary - 50 min	00:6	University of Tartu), Juras Banys (University of	iy oi Latvi.), Juras Ba	a), marco Mirin unys (University of	10:50	Coffee	Coffee 10:50 - 11:20	11:20	10:30	G. Niklasson	10:30	L. Valkunas
Invited - 30 min			Vilnius)		X	Beta hall 1	X	Beta hall 2	10:50	E. Kotomin	10:50	A. Bandura
Oral - 20 min	9:20	Andr	Andreas Schreyer	eyer	11:20	V. Shur	11:20	A. Kareiva	11:10	A. Yaremchenko	11:10	G. Kunakova
	10:10	Christi	Christina Trautmann	mann	11:50	V. Shvartsman	11:50	S. Kulkova	11:30	Y. Zhukovskii	11:30	E. Trukhanova
Synchrotron and	11:00	Coffee	Coffee 11:00 - 11:30	11:30	12:20	E. Politova	12:10	A. Antuzevics	11:50	R. Bartali	11:50	G. Gorokhov
Neutron facilities	X	Beta hall 1	X	Beta hall 2	12:40	P. Czaja	12:30	E. Ryklina	12:10	Lunch	Lunch 12:10 - 13:00	13:00
Radiation effects &	11:30	K. Klementiev	11:30	R. Evarestov	13:00	P. Ščajev	12:50	I. Khmelevskaya	X	ł	Beta Hall	1
Scintilators	12:00	M. Kirm	12:00	Y.Zhydachevskyy	00.01	D Dalitie	13:10	B. Kodatski	13:00	W	Maija Kuklja	lja
Optical materials	12:30	A.Frenkel	12:30	V. Nagirnyi	07:01	K. Egillis	13:30	C. Saikaew	13:50	Pete	Peter Kazansky	ısky
Thin films	13:00	A. Anspoks	13:00	A. Trukhanov	13:50	Lunch	Lunch 13:50 - 14:50	14:50		Closing - Rector 6	of the Un	Closing - Rector of the University of Latvia
Ferroelectrics	13:20	M. Klepka	13:20	V. Kuzovkov	X	Beta hall 1	X	Beta hall 2	14:40	I. 1	l. Muiznieks,	ks,
Nanocomposites and	13:40	Lunch	Lunch 13:40 - 14:40	14:40	14:50	J. Banys	14:50	A. Sternberg		Conference c	hairman	Conference chairman A.Sternberg
ceramics	X	Beta hall 1	X	Beta hall 2	15:20	<u>A. Salak</u>	15:30	T. Plank	15.00	Coodbya vefrachmants 15:00 - 16:00	chmont	s 15:00 - 16:00
Electronic, photonic	14:40	A. Bagaturyants	14:40	E. Zschech	15:50	O. Malyshkina	15:50	V. Kisand	00.01	annar afannan		00.01 - 00.CT 6
and magnetic materials	15:10	<u>M. Popova</u>	15:10	L. Österlund	16:10	E. Makagon	16:10	A. Popov				
and devices	15:40	I. Norrbo	15:40	I. Oja Acik		Excursion & Conference dinner at	onfere	nce dinner at				
International	16:00	L. Trinkler	16:00	H. Seemen	16:40	the Riga Motor Museum	Motor 1	Museum				
cooperation projects	16:20	J. Spigulis	16:20	M. Zubkins		16:4	16:40 - 21:30	30				
Energy	16:40	Photo &Coffee & Snacks 16:40 - 17:20	& Snack	s 16:40 - 17:20								
Nanomaterials	17:20	Poster session 17:20 - 19:00	ion 17:2	20 - 19:00								

International Conference Functional Materials and Nanotechnologies 'FMNT – 2018' PROGRAM

		Tuesday,	October 2
16:00 – 17:00	REGISTRATION		
17:00 – 18:30	WELCOME PARTY		
		Wednesday,	October 3
08:00 - 08:50	REGISTRATION		
		BETA HALL	
Beta hall	OPENING		
Chairperson: A	ndris Sternberg		
09:00 – 09:05	Andris Sternberg	Chairman of the Conference, Institute of Solid Sta ics, University of Latvia	te Phys-
09:05 – 09:10	Dmitrijs Stepanovs	Deputy State Secretary and Director of the Highe tion, Science and Innovation Department at Minis Education and Science, Latvia	
09:10 - 09:13	Valdis Segliņš Vice Rector – University of Latvia, Latvia		
09:13 - 09:16	Marco Kirm	Professor – Institute of Physics, University of Tartu	, Estonia
09:16- 09:19	Jūras Banys	Professor – Faculty of Physics, Vilnius University, L	ithuania
Beta hall	PLENARY SESSION		
09:20 – 10:10	Andreas Schreyer	ESS and Its Contributions to Future Functional Materials and Nanotechnology	PL-1
10:10 - 11:00	Christina Trautmann	Material Science and Nanostructures Produced with GeV Heavy lons	PL-2
11:00 – 11:30	COFFEE	•	
	•	BETA HALL 1	
Beta hall 1 SYNCHROTRON AND NEUTRON FACILITIES			
Chairperson: J	iri Kulda		
11:30 – 12:00	Konstantin Klementiev	MAX IV Laboratory in Lund, Sweden: Research Portfolio, Present Status Expected Performance	INV-1
12:00 – 12:30	Marco Kirm	A Role of Large Scale Facilities in the Develop- ment of Novel Functional Materials	INV-2
12:30 – 13:00	Anatoly Frenkel	A Neural Network Approach for Structural Char- acterization of Metal Nanoparticles and Clusters	INV-3
13:00 – 13:20	Andris Anspoks	Temperature Dependent Local Atomic Structure Studies of Bulk and Nanocrystalline CuO Using X-ray Absorption Spectroscopy	OR-1
13:20 – 13:40	Marcin Klepka	Studies of Non-crystalline Metal-organic Ligand Complexes Using Methodology Based on XAFS	OR-2

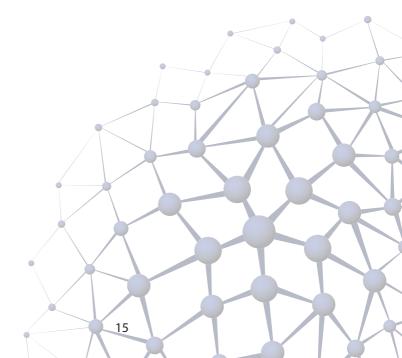
		Wednesday, October 3			
		BETA HALL 2			
Beta hall 2	RADIATION EFFECTS 8	SCINTILLATORS			
Chairperson: Eug	jene Kotomin				
11:30 – 12:00	Robert Evarestov	Theoretical Modeling of Point Defects in Crystals	INV-4		
	Yaroslav Zhydachevskyy	Photoluminescence Quantum Yield as a Test of Quantum Cutting Processes in Down-Convert- ing Phosphors	INV-5		
12:30 – 13:00	Vitali Nagirnyi	New Features of Hot Intraband Luminescence for Fast Timing	INV-6		
13:00 - 13:20	Alex Trukhanov	New Functional Material for Semiconductor Devices Protection against Electron Radiation	OR-3		
13:20 – 13:40	Vladimir Kuzovkov	Understanding of the Kinetics of Defect Anneal- ing in Heavily Irradiated Binary and Complex Oxides – Disordering Effects	OR-4		
13:40 – 14:40	LUNCH				
		BETA HALL 1			
Beta hall 1	OPTICAL MATERIALS				
Chairperson: Vita	li Nagirnyi				
	Alexander Bagatyurants	Theoretical Modelling in Nanophotonics	INV-7		
15:10 – 15:40	Marina Popova	Crystals for Optical Quantum Memory	INV-8		
15:40 – 16:00	Isabella Norrbo	Luminescence in Synthetic Hackmanites	OR-5		
16:00 – 16:20	Laima Trinkler	280 nm Emission Band in LiGaO ₂	OR-6		
16:20 – 16:40	Janis Spigulis	Human Skin as an Optical Material	OR-7		
BETA HALL 2					
Beta hall 2 THIN FILMS					
Chairperson: Juri	s Purans				
14:40 – 15:10	Ehrenfried Zschech	Application of X-ray Microcopy in Materials Science and Nanotechnology	INV-9		
15:10 – 15:40	Lars Österlund	Novel Self-Cleaning, Air Cleaning and Thermo- chromic Films for the Built Environment	INV-10		
15:40 – 16:00	Ilona Oja Acik	Photocatalytic TiO2 Thin Films for Air Cleaning Applications	OR-8		
16:00 – 16:20	Helina Seemen	The Properties of Atomic Layer Deposited Zirco- nium and Cobalt Oxide Nanolaminates	OR-9		
16:20 – 16:40	Martins Zubkins	Thin Film Deposition by Magnetron Sputtering at Cryogenic Substrate Temperatures	OR-10		
16:50 – 17:20	PHOTO & COFFEE & SM	IACKS			
17:20 – 19:00	POSTER SESSION				

Thursday, October 4			
08:30 - 09:00	REGISTRATION		
		BETA HALL	
09:00 - 09:10	TECHNICAL INFORMAT	ION	
Beta hall	PLENARY SESSION		
Chairperson: A	ndris Sternberg	· · · · · · · · · · · · · · · · · · ·	
09:10 – 10:00	Andrei Kholkin	Nanoscale Piezoelectric Materials: Structure, Properties, Applications	PL-3
10:00 – 10:50	Aharon Gedanken	Making the Hospital a Safer Place by the Sono- chemical coating of all its Textiles and Medical Devices with Antibacterial Nanoparticles	PL-4
10:50 – 11:20	COFFEE		
		BETA HALL 1	
Beta hall 1	FERROELECTRICS		_
Chairperson: Ju	ıras Banys		
11:20 – 11:50	Vladimir Shur	Shapes of Isolated Domains in Uniaxial Ferroe- lectrics	INV-11
11:50 – 12:20	Vladimir Shvartsman	Electrocaloric Effect in Barium Titanate Based Ceramics and Single Crystals	INV-12
12:20 – 12:40	Ekaterina Politova	Lead-free Ceramics on the Base of Sodium-Bis- muth Titanate and Sodium-Potassium Niobate	OR-11
12:40 – 13:00	Piotr Czaja	Influence of Powder Grinding Time on the Microstructure of the Lead-free K _{0.5} Bi _{0.5} TiO ₃ Ceramics	OR-12
13:00 – 13:20	Patrik Ščajev	Dispersion Carrier Recombination and Diffusion in MAPbl ₃ and MAPbBr ₃ Perovskite Crystals in Wide Excitation Range	
13:20 – 13:40	Roberts Eglitis Ab initio Calculations of ABO ₃ Perovskite (001), (011) and (111) Surfaces, Interfaces and Defects Therein		
	•	BETA HALL 2	
Beta hall 2	NANOCOMPOSITES A	ND CERAMICS	
Chairperson: A	natoly Frenkel		
11:20 – 11:50	Aivaras Kareiva	Multicomponent Metal Oxide Systems for Opti- cal and Magnetic Applications	INV-13
11:50 – 12:10	Svetlana Kulkova	Oxygen Diffusion in Ti-Al Alloys	OR-15
12:10 – 12:30	Andris Antuzevics	Electron Paramagnetic Resonance in Glass Ceramics	OR-16
12:30 – 12:50	Elena Ryklina	Effect of Grain Size on Microstructure, Transfor- mation Behavior and Functional Properties of Ti-Ni Shape Memory Alloy	OR-17

Thursday, October 4				
		BETA HALL 2		
12:50 – 13:10	Irina Khmelevskaya	Features of Nanostructure and Functional Prop- erties Formation in Ti-Ni SMA by ECAP Method Under Quasi-continuous Mode	OR-18	
13:10 – 13:30	Bogdan Kodatski	Nematic Mesomorphous Systems Based on Dispersions of Carbon Nanotubes and Mineral Particles	OR-19	
13:30 – 13:50	Charnnarong Saikaew	Influences of Sputtering Process Factors on Wear Resistance of TiN Coated on a Machine Component	OR-20	
13:50 – 14:50	LUNCH			
		BETA HALL 1		
Beta hall 1	ELECTRONIC, PHOTON	NIC AND MAGNETIC MATERIALS AND DEVICES		
Chairperson: Ar	ndrei Kholkin			
14:50 – 15:20	Jūras Banys	Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers	INV-14	
15:20 – 15:50	Andrei Salak	Tuneable Magnetic Co(II)-Containing Layered Double Hydroxides	INV-15	
15:50 – 16:10	Olga Malyshkina	Determination of the Electron Effective Mass for n-type Germanium by the Low-frequency Impedance	OR-21	
16:10 – 16:30	Evgeniy Makagon	Ceria-based electro-chemo-mechanical actua- tor with Ti/Ce1×GdxO2-x/2 composite contacts	OR-22	
BETA HALL 2				
Beta hall 2 INTERNATIONAL COOPERATION PROJECTS				
Chairperson: Ma	arco Kirm			
14:50 – 15:10	Andris Sternberg	CAMART ² - Regional Development Opportunity	OR-23	
15:10 – 15:30	Toomas Plank	Solar Energy with New Generation Power Elec- tronics Solutions	OR-24	
15:30 – 15:50	Kisand Vambola	Baltic TRAM – a Network of Industrial Research Centers Providing Analytical Services for Business Innovation in the Baltic Sea Region	OR-25	
15:50 – 16:10	Anatoli Popov	Advanced Materials and Technologies in Fusion Research: An Overview and Some Recent Results from Latvian EUROfusion Laboratory	OR-26	
16:40 – 21:30	EXCURSION AND CON	FERENCE BANQUET AT THE RIGA MOTOR MUSE	JW	

Friday, October 5				
09:00 - 09:30	REGISTRATION & COFFE	E		
BETA HALL 1				
Beta hall 1	ENERGY			
Chairperson: Ma	artins Rutkis			
09:30 –10:00	Jens Pflaum	Low-Dimensional Organic Conductors for Ther- moelectric Applications	INV-16	
10:00 – 10:30	Luciana Vieira	Functional Materials for the CO ₂ -based Elec- trosynthesis of Ethylene Oxide	INV-17	
10:30 – 10:50	Gunnar A. Niklasson	Impedance Spectroscopy of Water Splitting Re- actions on Nanostructured Metal-based Catalysts	OR-27	
10:50 – 11:10	Eugene Kotomin	First Principles Calculations of Perovskite Solid Solutions for Fuel Cells	OR-28	
11:10 – 11:30	Aleksey Yaremchenko	LaNiO₃-based Oxygen Electrodes for Solid Oxide Electrolysis Cells	OR-29	
11:30 – 11:50	Yuri Zhukovskii	First Principles Evaluation of Photocatalytic Suitability of 2H Structured and [0001] Oriented Graphene-like WS2 Nanosheets and Nanotubes	OR-30	
11:50 – 12:10	Ruben Bartali	Hydrogen Production by Water-Hydrolysis using Graphene Powder Coated with Magnesium	OR-31	
12:10 – 13:00	LUNCH			
		BETA HALL 2		
Beta hall 2	NANOMATERIALS			
Chairperson: Ko	onstantin Klementiev			
09:30 –10:00	Andrey Lipovskii	Plasmonic Nanoislands on Glass: Formation and Properties	INV-18	
10:00 – 10:30	Mitch Chou	Nitch Chou Preparation and Characterization of Heteroep- itaxial Cu ₂ O Thin Film and Devices on Metallic Substrates INV-19		
10:30 – 10:50	Leonas Valkunas	Relaxation Pathways in Semiconducting Carbon Nanotubes	OR-32	
10:50 – 11:10	:50 – 11:10 Andrei Bandura New Three-body Force-field for Calculation of OR-33 the Thermodynamic Properties of MoS ₂ Nano- layers and Nanotubes		OR-33	
11:10 – 11:30	Gunta Kunakova	Studies of Magnetotransport and Josephson Supercurrent in Topological Insulator Nanorib- bons	OR-34	
11:30 – 11:50	Ekaterina Trukhanova	Synthesis and Magnetotransport Properties of the Multilayered Quasi-one-dimensional Nanostructures	OR-35	
11:50 – 12:10	Gleb Gorokhov	Carbon Nanotubes vs Graphene Nanoplatelets for 3D-printable Composites	OR-36	
12:10 – 13:00	LUNCH			

		Friday,	October 5		
		BETA HALL			
Beta hall	PLENARY SESSION				
Chairperson: An	ndris Sternberg				
13:00 – 13:50	Maija Kuklja	Understanding Chemical Reactions Triggered by Defects on Energetic Materials and Interfac- es. Insight from Quantum Chemistry	PL-5		
13:50 – 14:40	Peter Kazansky	Advancing the art of femtosecond laser writing	PL-6		
Beta hall	Beta hall CLOSING OF THE CONFERENCE				
14:40 – 14:50	4:50 Indrikis Muiznieks Rector of the University of Latvia				
14:50 – 15:00	Andris Sternberg	Chairman of the Conference, Institute of Solid Sta ics, University of Latvia	ate Phys-		
15:00 – 17:00	GOODBYE REFRESHM	ENTS			



PO-1 Comparative First-Principles Calculations of ZrS2 and HfS2- based Nanotubes Anton Domnin PO-2 Comparative Study of Phonons and Thermodynamic Prop- eries of MoS2 and WS5 Nanotubes Robert Evarestov; Andrei Bandura PO-3 Atomistic Scale Modelling of Modern Materials using ACELAN Package Roman Gruzdev PO-4 Pine Influence of Impurities on the Formation Energies of Structure of InSb(111) Surface Alexander Bakulin PO-5 Influence of Fluorine and Oxygen Adsorption on Electronic Structure of InSb(111) Surface Denis Gryaznov PO-6 CO ₂ Adsorption on Mixed Ionic-Electronic Conducting Membranes Denis Gryaznov PO-7 Negative Thermal Expansion of ScF3: First Principles vs Empirical Molecular Dynamics Dmitry Bocharov PO-8 Simulation of the Band Structure and Density of States of He Nanocrystal NaCl Lyudmila Myasnikova PO-9 First Principles Calculations for Polar YAIO3 (001) Surfaces Roberts Eglitis PO-10 Quantum Paraelectric State in (Pby5n-y)aPx5a Crystals Ilona Zamaraite PO-11 Modelling of F-type Centers Thermal Annealing in Neutron Irradiated and Thermochemically Reduced BeO Vladimir Kuzovkov PO-13 Structural and Electronic Properties of AbG9/TiaAl Interface Sergey S. Kulkov <t< th=""><th></th><th>POSTER PRESENTATIONS</th><th></th></t<>		POSTER PRESENTATIONS	
based Nanotubes Number of Phonons and Thermodynamic Properties of MoS₂ and WS₁ Nanotubes Robert Evarestov; Andrei Bandura PO-3 Atomistic Scale Modelling of Modern Materials using ACELAN Package Roman Gruzdev PO-4 The Influence of Impurities on the Formation Energies of Point Defects in Ti-Al Alloys Alexander Bakulin PO-5 Structure of InSp(111) Surface Artem Fuks PO-6 C0₂ Adsorption on Mixed Ionic-Electronic Conducting Membranes Denis Gryaznov PO-7 Negative Thermal Expansion of ScFa: First Principles vs Empirical Molecular Dynamics Dmitry Bocharov PO-8 Simulation of the Band Structure and Density of States of the Nanocrystal NaCl Lyudmila Myasnikova PO-9 First Principles Calculations for Polar YAIO₃ (001) Surfaces Roberts Eglitis PO-10 Quantum Paraelectric State in (PbySn:-y):P2:Sa Crystals Ilona Zamaraite PO-11 Modeling of F-type Centers Thermal Annealing in Neutron Irradiated and Thermochemically Reduced BeO Valatimir Kuzovkov PO-12 Lattice Dynamics of White Phosphorus Janis Brokans PO-13 Structural and Electronic Properties of ALOa/Ti:Al Interface Sergey S. Kulkov PO-15 Ab Initio Simulation of (Ba,Sr/Ca)TIO ₃ Composite Per- ovskites			
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