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INTRODUCTION

Who would have thought at the beginning of the global economic crisis in 2009 that in 2013 Slovenia would not only be facing even more serious problems, but would also still be looking for solutions to the same challenges set before us back then? I cannot say that in recent years the state has not made an effort to change the economic trends for the better. We have seen a lot of sensible, and also foolish, attempts at tackling the problems; however, so far nobody has managed to put into place the systemic and comprehensive structural reforms that Slovenia needs. So I am writing this introduction to the Institute's Annual Report for the fifth time in succession thinking about the times Slovenia is facing due to the crisis that is crippling the economy and all the other social activities, among which science and technological development also suffer from its consequences. Here it is necessary to point out that, at least at the beginning of the crisis, there was a belief that knowledge and research were of key importance for a developmental breakthrough in Slovenia; however, later this belief faded away to the extent that scientific and technological research were the areas most significantly affected by the flat cuts in the public sector. Such conduct is not in line with the guidelines of the European Commission that, in 2012 in its annual review, appealed for a smart fiscal consolidation with the priority areas that stimulate growth, such as investments into research and development, the acquisition of knowledge and education, that are crucial for the knowledge-based economy that will be competitive and will provide new jobs in the future.



Prof. Jadran Lenarčič, Director of the Jožef Stefan Institute

Slovenia will have to continue to take out loans, not in order for us to remain as we are now, to keep doing what we already do, not to keep avoid doing what we do not want to do, to maintain our standards and current habits, but to increase our productivity in all areas and, above all, to boost the economy, allowing it to make a breakthrough to a higher technological level. It is easy to calculate that Slovenia could be one of the rich countries if all the country's workers increased their productivity (or added value) by twenty-five minutes each working day or by three minutes each working hour. When we see our crisis from this angle, it does not seem to be unsolvable, as it would clearly be enough if those who obstruct others in their efforts simply stopped behaving in this way. This simplification is perhaps exaggerated, but it only appears to be naive, as it basically shows us that, to a large extent, our society failed with regard to moral values and assessments, and a change in this respect could also lead to structural and economic changes. Or vice-versa, without the change in the values and assessments, especially in the area of knowledge and creativity, no crucial structural reforms and new economic drive can be expected.

I believe that the main aim of all our efforts should be finding a way to create new knowledge and ideas, and integrating them in economic and social developments. Such an attitude would take us beyond the current "accounting" concept of managing the country, placing creativity and knowledge at the centre of our attention. Slovenia simply should not be managed only in view of a flat-rate reduction of costs; instead we should create an environment in which different skills and motives can meet, in which research and entrepreneurship find each other, in which we find the courage and desire to be the first to accomplish something new and big, and in which the capital can support such efforts, so opening up new opportunities. Ideas are like seeds that only grow in an appropriate environment. However, in spite of the relatively modest working conditions, the Institute still manages to succeed, with its excellent results in many areas, in a competition with some of the richest research players in the international sphere.

Prof. Jadran Lenarčič Director of the Jožef Stefan Institute

A BRIEF HISTORY OF THE JOŽEF STEFAN INSTITUTE

1946

 Decision taken by the Slovenian Academy of Science and Arts to build a Physics Institute

1949

 Research connected to the peaceful use of atomic energy started, financed by the Federal Government

1952

 Institute renamed the Jožef Stefan Physics Institute and moved to new laboratories on its present site

1954

 The betatron and an electron microscope installed as the institute's first major pieces of equipment

1956

- Van de Graaff accelerator, constructed at the institute, started operation
- 1958
- Institute reorganised and new fields of activity defined: nuclear physics, solidstate physics, chemistry, and radiobiology

1959

 Institute renamed the Jožef Stefan Nuclear Institute. The major source of income was provided by the Yugoslav Atomic Energy Commission



Mass spectrometer at the JSI (about 1960)

1962

One of the first compounds of a noble gas, XeF₆, synthesised at the institute The first computer for research, ZUSE Z 23, installed

1966

Nuclear research reactor TRIGA starts operation

1968

Yugoslav Atomic Energy Commission ceases to operate; The Republic of Slovenia becomes the institute's dominant source of research funding

1969

Institute is renamed as the Jožef Stefan Institute

1970

University of Ljubljana becomes a co-founder of the Jožef Stefan Institute, together with the Federal Executive Council

1971

A new unit, INOVA, established with the aim of applying the institute's expertise and output to productive use in the national economy



Institute buildings after the opening in 1953

1972

 New computer Cyber 72 purchased, and the Republic Computer Centre established as an independent unit of the Jožef Stefan Institute

1974

- Collaboration with the international centre CERN in the field of high-energy physics started
- SEPO group for evaluating environmental interventions is established

1976

First Yugoslav 8-bit processor computer DARTA 80

1979

- Contract defining cooperation between the Jožef Stefan Institute and the Nuclear Power Plant Krško is signed
- First robot in Slovenia is constructed

1982

 Ecological Laboratory with Mobile Unit established as a special unit of the Slovenian Civil Protection Organisation

1983

 Stefin, a cysteine proteinase inhibitor named after Jožef Stefan, isolated and its primary structure determined



The Reactor Centre, Podgorica, built in 1966

1985

- "2000 New Young Researchers" project established by the Slovenian Research Council
- Centre for Hard Coatings established by the Jožef Stefan Institute and the firm SMELT

1987

 INEA established by the Jožef Stefan Institute as an independent company to promote technology transfer in the fields of cybernetics and energy management



Nuclear magnetic resonance spectrometer

1989

 Milan Čopič Nuclear Training Centre established 1990

- The first Slovenian supercomputer, CONVEX, installed at the Jožef Stefan Institute 1992
- \sim New technology centres established by the Ministry of Science and Technology
- Jožef Stefan Institute restructured by the Slovenian Government as a public research institution
- Jožef Stefan Technology Park founded, later to become the Ljubljana Technology Park

1995

- Jožef Stefan Institute is a co-founder of the international postgraduate school for environmental sciences, the Nova Gorica Polytechnic
- \sim $\;$ Research institutes in Velenje, ERICo and Valdoltra established by the Institute $\;$
- 1997
- $\sim \quad 3.5 \text{-MeV electrostatic accelerator, TANDETRON, installed}$

1999

~ Jožef Stefan Institute celebrates its 50th anniversary

2003

 \sim Jožef Stefan International Postgraduate School established

2004

 Jožef Stefan Institute is chosen as the coordinator of four Research Centres of Excellence

2007

- nanomanipulation of single atoms using low-temperature scanning tunneling microscope
- New ERDA/RBS beamline installed at the TANDETRON accelerator at the Microanalytical center



The beginnings of robotics at the JSI, in 1985

FORMER DIRECTORS



Prof. Anton Peterlin, Founder and first Director of the Jožef Stefan Institute, 1949–1955 Karol Kajfež, 1955–1958 Lucijan Šinkovec, B. Sc., 1959–1963 Prof. Milan Osredkar, 1963–1975 Prof. Boris Frlec, 1975–1984 Prof. Tomaž Kalin, 1984–1992 Prof. Danilo Zavrtanik, 1992–1996 Prof. Vito Turk, 1996–2005

Prof. Anton Peterlin, first Director of the Jožef Stefan Institute

ORGANISATION OF THE JOŽEF STEFAN INSTITUTE

BOARD OF GOVERNORS

DIRECTOR

SCIENTIFIC COUNCIL

RESEARCH DEPARTMENTS

Physics

Theoretical Physics (F-1) Prof. Svjetlana Fajfer Low and Medium Energy Physics (F-2) Asst. Prof. Matej Lipoglavšek Thin Films and Surfaces (F-3) Dr. Peter Panjan Surface Engineering and Optoelectronics (F-4) Prof. Miran Mozetič Solid State Physics (F-5) Prof. Igor Muševič Complex Matter (F-7) Prof. Dragan Dragoljub Mihailović **Reactor Physics (F-8)** Asst. Prof. Andrej Trkov **Experimental Particle Physics (F-9)** Prof. Marko Mikuž

Chemistry and Biochemistry

Inorganic Chemistry and Technology (K-1) Asst. Prof. Gašper Tavčar Physical and Organic Chemistry (K-3) Prof. Ingrid Milošev Electronic Ceramics (K-5) Prof. Marija Kosec Engineering Ceramics (K-6) Prof. Tomaž Kosmač Nanostructured Materials (K-7) Prof. Spomenka Kobe Synthesis of Materials (K-8) Prof. Darko Makovec Advanced Materials (K-9) Prof. Danilo Suvorov Biochemistry, Molecular and Structural Biology (B-1) Prof. Boris Turk Molecular and Biomedical Sciences (B-2) Prof. Igor Križaj Biotechnology (B-3) Prof. Janko Kos Environmental Sciences (O-2) Prof. Milena Horvat

Electronics and Information Technology

Automation, Biocybernetics and Robotics (E-1) Asst. Prof. Leon Žlajpah Systems and Control (E-2) Dr. Vladimir Jovan Artificial Intelligence Laboratory (E-3) Prof. Dunja Mladenić **Open Systems and Networks (E-5)** Prof. Borka Jerman Blažič **Communication Systems (E-6)** Asst. Prof. Mihael Mohorčič **Computer Systems Department (E-7)** Prof. Franc Novak Knowledge Technologies (E-8) Prof. Nada Lavrač Intelligent Systems (E-9) Prof. Matjaž Gams

Reactor Techniques and Energetics

Reactor Engineering (R-4) Prof. Leon Cizelj

CENTRES

Reactor Centre (RIC) Prof. Borut Smodiš Centre for Networking Infrastructure (CNI) Vladimir Alkalaj, M. Sc. Science Information Centre (SIC) Dr. Luka Šušteršič **Energy Efficiency Centre (EEC)** Stane Merše, M. Sc. Centre for Knowledge Transfer in Information Technologies (CT-3) Mitja Jermol, M. Sc. Milan Čopič Nuclear Training Centre (ICJT) Prof. Igor Jenčič Centre for Electron Microscopy (CEM) Prof. Miran Čeh Centre for Technology Transfer and Innovation (CTT) Dr. Špela Stres Microanalytical Instrumental Centre (MIC) Asst. Prof. Primož Pelicon Combined Atomic Microscope (UHV-AFM/STM) Prof. Maja Remškar

Helium Liquifier with Superconducting Magnet and Helium Regeneration System Milan Rožmarin, B. So Mass Spectrometry Centre Dr. Dušan Žigon National Centre for Microstructure and Surface Analysis Prof. Miran Čeh National Centre for High Resolution NMR Spectroscopy Prof. Janez Dolinšek **Centre for Protein Structure** Prof. Dušan Turk Nanolitography and Nanoscopy Prof. Dragan Mihailović **Centre for Experimental Particle Physicis** in International Laboratories Prof. Marko Mikuž Hot Cells Facility Asst. Prof. Borut Smodiš Video-conferencing Centre Prof. Borka Jerman Blažič

ADMINISTRATION, SERVICES AND SUPPORT UNITS

Administration and Services

Legal and Personnel (U-2) Katja Novak, LL. B. Sales and Purchase Department (U-3) Darko Korbar, M. Sc., MBA Finance and Accounting (U-4) Regina Gruden, B. Econ. Public Relations Polona Strnad, B. Sc. Technical Services (TS) Aleš Cesar, B. Sc.

Support Units

Radiation Protection Unit (SVPIS) Matjaž Stepišnik, M. Sc. Quality Assurance (QA) Ljubo Fabjan, M. Sc. Centre for Business Applications (CPO) Mato Nowak, B. Sc. Workshops Bogdan Veber, B. Sc.

PARTICIPATION IN THE REGIONAL DEVELOPMENT OF RESEARCH

	Technology Centres							
Ljubljana Technology Park Ltd.	Technology Centre for Circuits, Components, Materials, Technologies and Equipment for Electrotechnic (TC SEMTO)	Technology Centre for Production Automation, Robotics and Informatics (ARI)						
University of Nova Gorica	Nanotesla Institute Ljubljana	Security Technology						
Jožef Stefan International	Development Centre for Hydrogen	Competence Centre (SETTCE)						
Postgraduate School	Technologies							
	Centres of Excellence							
Nanocenter - Center of Excellence in Nanoscience and Nanotechnology	Centre of Excellence NAMASTE	CEBIC Centre of Excellence for Biosensors, Instrumentation and Process Control						
Centre of Excellence for Integrated	Centre of Excellence for Polymer Materials and Technologies (PoliMaT)	CO NOT: Centre of Excellence for Low- Carbon Technologies						
of Proteins (CIPKeBiP)	EN-FIST Centre of Excellence	Centre of Excellence for Space Sciences and Technologies SPACE-SI						

MANAGEMENT

DIRECTORATE

Director JSI Prof. Jadran Lenarčič

Advisers Jože Kašman, B. Sc. Dr. Boris Pukl Marta Slokan, LL. B.

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STAFF QUALIFICATIONS

1949-2012



RECIPIENTS OF THE JSI AWARDS AND TITLES

HONORARY MEMBERS

Prof. Robert Blinc⁺, President of the Scientific Council of the Jožef Stefan Institute from 1992 to 2007 (1933 - 2011)

Prof. Jean-Marie Dubois, Institut Jean Lamour, CNRS - Centre National de la Recherche Scientifique, Paris and Université Lorraine, Nancy, France

Prof. Boris Frlec, Director of the Jožef Stefan Institute from 1975 to 1984

Prof. Robert Huber, Nobel Prize Winner, Max-Planck-Institut für Biochemie, Munich, Germany

 $\label{eq:prof.Milan Osredkar^{\oplus}, Director of the Jožef Stefan Institute from 1963 to 1975 (1919 - 2003) \\ \mbox{Prof. Anton Peterlin^{\oplus}, Founder and First Director of the Jožef Stefan Institute from }$

1949 to 1955 (1908 - 1993)

ASSOCIATE MEMBERS

Prof. David C. Ailion, University of Utah, Salt Lake City, Utah, USA
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Prof. John H. Beynon, University of Wales Swansea, Swansea, United Kingdom
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Dresden, Germany

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Prof. James W. Cronin, Nobel Prize Winner, University of Chicago, Chicago, Illinois, USA Prof. Richard Ernst, Nobel Prize Winner, ETH Zurich, Switzerland

- $\label{eq:problem:problem} \textbf{Prof. Robert Huber}, \textit{Nobel Prize Winner}, \textit{Max-Planck-Institut}, \textit{Martiensried}, \textit{Germany}$
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- Prof. Børge Diderichsen, Novo Nordisk, Bagsvaerd, Denmark
- Prof. Jean Etourneau, Institut de Chimie de la Matière Condensée de Bordeaux, CNRS, Pessac, France

- Prof. Reinosuke Hara, Seiko Instruments, Tokyo, Japan
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- Prof. Dietrich Munz, Universität Karlsruhe, Karlsruhe, Germany
- Prof. Günther Petzow, Max-Planck-Institut für Metallforschung, Stuttgart, Germany
- Prof. Bernard Roth, Stanford University, Stanford, California, USA
- Prof. John Ryan, University of Oxford, Oxford, United Kingdom
- Prof. Volker Sörgel, Ruprecht-Karis-Universität, Heidelberg, Germany Prof. H. Eugene Stanley, Boston University, Boston, Massachusetts, USA Prof. Thomas Walcher, Universität Mainz, Mainz, Germany

DELEGATIONS AND VISITORS

Dr.Mark Pleško, Director, Cosylab d.d., Ljubljana, 13 January 2012 Dr. Edvard Kobal, Director, The Slovenian Science Foundation, Ljubljana, 2 February 2012 Ambassador of India, Embassy of India, Vienna, Austria, 3 February 2012 Dr. Boris Pleskovič, President, Slovenian World Congress, Ljubljana, 7 March 2012 Prof. Rudi Grimm, University of Innsbruck, Innsbruck, Austria, 19 March 2012

- H. E. Mrs Rossella Franchini Sherifis, Ambassador of Italy, Embassy of Italy, Ljubljana, 29 March 2012
- Delegation of Ambassadors of the Republic of Slovenia, 10 April 2012
- H. E. Mr Mohammad Rahim Aghaeipour, Ambassador of the Islamic Republic of Iran, Embassy of the Islamic Republic of Iran, Ljubljana, 18 April 2012
- H. E. Mr Paul Jansen, Ambassador of the Kingdom of Belgium, Embassy of the Kingdom of Belgium, Ljubljana, 18 April 2012
- Mrs Maire Geoghegan-Quinn, Member of the European Commission for Research, Innovation and Science, European Commission, Brussels, Belgium, 25 April 2012
- H. E. Mr Gilberto Fonseca Guimarăes de Moura, Ambassador of the Federative Republic of Brazil, Embassy of the Federative Republic of Brazil, Ljubljana, 5 June 2012
- Dr. Matjaž Godec, Institute of Metals and Technology, Ljubljana, 11 June 2012
- H.E. Ms Alenka Suhadolnik, MA, Ambassador of the Republic of Slovenia, Embassy of the Republic of Slovenia, Tel Aviv, Israel, 15 June 2012
- H. E. Mr Marius Cosmin Boiangiu, Ambassador of Romania, Embassy of Romania, Ljubljana, 17 July 2012
- Dr. Robert Ferko, 18 July 2012
- H. E. Mr Pierre-Francois Mourier, Ambassador of the French Republic, Embassy of the French Republic, Ljubljana, 19 September 2012
- Mateja Dermastja, M. Sc., CEO, PoliMaT Centre of Excellence, Ljubljana, 27 September 2012
- Prof. Boris Frlec, Former Director of JSI, Ljubljana, 25 October 2012
- Prof. Oh In Kwon, Prof. Eung Je Woo, Prof. Jin Keun Seo, Konkuk University, Korea Kyung Hee University, Suwona, Korea Yonsei University, Seoul, Korea, 25 November 2012



Rudi Grimm

INTERNATIONAL COOPERATION

Multilateral international cooperation	No. of projects
7. FP (COOPERATION: HEALTH, FOOD, AGRICULTURE/FISHERIES, BIOTECHNOLOGY, INFORMATION COMMUNICATION TECHNOLOGIES, NANOSCIENCES + NANOTECHNOLOGIES, MATERIALS + NEW PRODUCTION TECHNOLOGIES, ENERGY, ENVIRONMENT AND CLIMATE CHANGE, TRANSPORT (INCLUDING AERONAUTICS), SOCIO-ECONOMIC SCIENCES + THE HUMANITIES, SPACE, SECURITY; IDEAS: FRONTIER RESEARCH (EUROPEAN RESEARCH COUNCIL); PEOPLE: MARIE CURIE FELLOWSHIPS; CAPACITIES: RESEARCH INFRASTRUCTURES, SMES, REGIONS OF	94
KNOWLEDGE, RESEARCH POTENTIAL, SCIENCE AND SOCIETY, INCO (HORIZONTAL), DEVELOPMENT OF POLICIES)	
7. FP - EURATOM	44
6. FP	3
ESRR	5
OTHERS (COST, IAEA, EIE, IRMM, ESA, NATO, CIP, CE, SEE, EMRP, WHO, LIFE+)	107
TOTAL	253

Bilateral cooperation	No. of projects
Argentine	3
Austria	3
Bulgaria	2
Brazil	3
Montenegro	3
Cyprus	1
Czech Republic	1
Finland	2
France	15
Croatia	7
Italy	2
Japan	7

Bilateral cooperation	No. of projects
China	5
Korea	2
Hungary	2
Norway	2
Romania	4
Russia	2
Slovakia	1
Serbia	6
Turkey	1
Ukraine	1
USA	24
TOTAL	99

INTERNATIONAL COOPERATION AGREEMENTS

In 2012, cooperation agreements were signed between the Jožef Stefan Institute and:

- 1. TRL Technology Limited, Gloucestershire, United Kingdom (F2, E6)
- 2. ENEA UTFUS, Frascati (RM), Italy (F8)
- 3. Porzellanfabrik Frauenthal, Frauenthal, Austria (K1)
- Institute of Physical Chemistry "Ilie Murgulescu" of Romanian Academy, Bucharest, Romania (K5)
- 5. Du Pont (U.K.) Limited, Hertfordshire, United Kingdom (K5)
- 6. Tele and Radio Research Institute (ITR), Warsaw, Poland (K5)
- 7. American Type Culture Collection ATCC, Manassas, VA, USA (B1)
- 8. F. Hoffmann-La Roche Ltd, Basel, Switzerland (B1)
- 9. Helmholtz Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Berlin-Adlershof, Germany (B1)

- 10. Zheijang University, State Environmental Protection Engineering Center for Coal-Fired Air Pollution Control (ZU SEPEC), Hangzhou, PR China; Jožef Stefan International Postgraduate School (IPS), Ljubljana, Slovenia (O2)
- 11. Comenius University Bratislava, Faculty of Mathematics, Physics and Informatics, Bratislava, Slovak Republic (O2)
- 12. Fundación Universidad Empresa ADEIT, Departamento de Teleformación/ Leonardo da Vinci, Valencia, Spain (O2)
- 13. Tampere University of Technology, Department of Production Engineering, Tampere, Finland (E1)
- 14. Hellenic Military Academy, Athens, Greece (E1)
- 15. Hexis AG, Winterthur, Switzerland; Hexis GmbH, Konstanz, Germany (E2)
- 16. The Université Pierre et Marie Curie (UPMC), Paris, France (E5)
- 17. Korea Atomic Energy Research Institute (KAERI), Daejeon, Korea (R4)

COOPERATION WITH UNIVERSITIES

FULL-TIME FACULTY MEMBERS

Professors

- 1. Asst. Prof. Denis Arčon, University of Ljubljana, Faculty of Mathematics and Physics
- 2. Prof. Iztok Arčon, University of Nova Gorica
- 3. Prof. Janez Bonča, University of Ljubljana, Faculty of Mathematics and Physics
- 4. **Prof. Ivan Bratko**, Academician, University of Ljubljana, Faculty of Computer and Information Science
- 5. Prof. Milan Brumen, University of Maribor, Faculty of Education
- 6. Prof. Dean Cvetko, University of Ljubljana, Faculty of Mathematics and Physics
- 7. Prof. Mojca Čepič, University of Ljubljana, Faculty of Education
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- 121. Asst. Prof. Leon Žlajpah, Jožef Stefan International Postgraduate School, Ljubljana
- 122. Asst. Prof. Bernard Ženko, Faculty of Information Studies, Novo Mesto and University of Nova Gorica
- 123. Asst. Prof. Martin Žnidaršič, Faculty of Information Studies, Novo Mesto and University of Nova Gorica

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- 32. Žerovnik Gašper, University of Maribor, Faculty of Energy Technology
- 33. Dr. Dušan Žigon, Jožef Stefan International Postgraduate School, Ljubljana

ART EXHIBITIONS AT THE JSI

Igor Banfi, 16 January-16 February Kamila Volčanšek, 20 February-15 March Bogdan Borčič, 19 March-12 April Seven Masters of Photography, 16 April-10 May Jernej Skrt, 14 May-14 June Miha Boljka, 18 June-12 July Ljubljana Fine Artist Society, 16 July-27 September Roman Makše, 15 October-15 November Lojze Logar, 26 November-17 January 2013



Prof. Jadran Lenarčič, Director of the JSI, and Bogdan Borčič at the opening of the exhibition of his works

INSTITUTE COLLOQUIA

15 January 2012: **Andrej Trkov** Jožef Stefan Institute *Nuclear data - and what to do with them*

25 January 2012: Viktor V. Kabanov Jožef Stefan Institute Superconductivity: Electron-phonon Coupling and Unconventional Pairing with Repulsive Interaction

15 February 2012: **Richard Dronskowski** RWTZ Aachen University, Aachen, Germany *Solid-state chemistry - where chemistry meets physics and materials science*

29 February 2012: **Maya Kiskinova** Elettra, Trieste, Italy **Selected research highlights and recent developments at Elettra Laboratory in Trieste**

19 March 2012: **Rudi Grimm** Universität Innsbruck, Innsbruck, Austria *Ultracold Atoms: Model Kits for Quantum Matter*

20 March 2012: **Boris Žemva** Jožef Stefan Institute *Half a century of noble gases chemistry: A historical overview, the developments in the world and the main achievements at "Jožef Stefan" Institute*

21 March 2012: Boris Turk

Jožef Stefan Institute, Centre of Excellence for Integrated Approaches in Chemistry and Biology of Proteins, Center of Excellence: Nanoscience and Nanotechnology and Faculty of Chemistry and Chemical Technology, University of Ljubljana *Biomedicine - Challenges for the Future*

23 March 2012: **Gabrijel Kernel** Jožef Stefan Institute, Faculty of Mathematics and Physics, University of Ljubljana *Development of elementary-particle physics*

4 April 2012: **Goran Senjanović** ICTP, Trieste, Italy *LHC and the neutrino paradigm*

18 April 2012: Alexey Ekaykin Arctic and Antarctic Research Institute, St. Petersburg, Russian Federation Drilling the Ice from the Past to the Future: The history of deep ice drilling at Antarctic Vostok Station and Lake Vostok exploration 25 April 2012: **Nikolaus Nestle** BASF, Ludwigshafen, Germany *Low-field NMR in industrial analytics*

9 May 2012: **Miran Mozetič** Jožef Stefan Institute *Surface modification with non-equilibrium plasma*

23 May 2012: **Igor Jenčič** Jožef Stefan Institute *Energy – numbers rather than emotions*

6 June 2012: **Stephan Herminghaus** Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany *Experiments with active emulsions*

22 June 2012: **Matjaž Gams** Jožef Stefan Institute *The centenary of Turing, the Einstein of computer science*

20 September 2012: **Murugappan Muthukumar** University of Massachusetts, Amherst, USA *Theory of macromolecular transport through protein channels and nanopores*

17 October 2012: **Bogdan Povh** Max Planck Institute for Nuclear Physics, Heidelberg, Germany *A somewhat nostalgic view of nuclear physics*

9 November 2012: **Jure Zupan** University of Cincinnati, Cincinnati, USA *What is the relevance of the discovery of Higgs boson?*

21 November 2012: **Griša Močnik** Aerosol d.o.o., Ljubljana *Measurement of aerosolized black carbon - Health and Climate - two birds with one stone?*

4 December 2012: **Steffen Krämer** Laboratoire National des Champs Magnétiques Intense, Grenoble, France *Physics, chemistry and materials science in very high magnetic fields: NMR and beyond*

12 December 2012: **Đani Juričić** Jožef Stefan Institute *Diagnostics, prognostics and e-maintenance of industrial systems*

FINANCING

REVENUES JSI (€) AND NUMBER OF PROJECTS

		Contribution		Contribution		No. of Projects
	2012	2012	2011	2011	Index 2012/2011	in 2012
National Agencies and Ministries	33,267,535	71.1 %	37,946,161	75.6 %	87.7	573
National Market	5,012,171	10.7 %	4,682,766	9.3 %	107.0	281
International Market	7,924,955	16.9 %	6,968,502	13.9 %	113.7	384
Other Revenues	585,646	1.3 %	601,959	1.2 %	97.3	
TOTAL	46,790,307	100.0 %	50,199,388	100.00 %	93.2	1238



POSTGRADUATES FINANCED

1985-2012





JSI UNDERGRADUATE SCHOLARSHIPS

1977-2012

Year]	FMF	FKKT	FKKT	NTF	FDV	FA	BF	FE and	Other	FG and	UNG	IPS	Total
	Physics		UNI LJ	UNI MB					FRI	UNI LJ	FERI			
1982	115	38	100						50	12				315
1983	10	1	5						9		1			26
1984	11	3	7					1	12		1			35
1985	18	4	6					1	19		1			49
1986	16	8	4						22	2				52
1987	20	8	4						23	2				57
1988	26	7	8					1	27	2				71
1989	26	6	10					1	19	3	1			66
1990	26	5	11					2	25		1			70
1991	23	2	9					2	24	2	1			63
1992	22	3	16					3	17	1				62
1993	21	1	15					3	13	1				54
1994	7	1	8					3	6					25
1995	2		9					3	5					19
1996	2		9					3	5					19
1997	2		12					1	4		1			20
1998	1		6					1	7		1			16
1999	2		7					4	7					20
2000	1		5					3	9					18
2001	3		13					3	10					29
2002	4		20					3	10					37
2003	3		18					2	12	1				36
2004	4		17					1	15	1	2	2		42
2005	3		12			1		2	19		2	1		40
2006	2		12			1		1	17		2	2		37
2007	3		14			1		2	18		2	1		41
2008	2	1	13	3		1		2	15		1	1		39
2009	2	1	17	4		1		5	16		1	2		49
2010	2		11	5	2	1	1	3	10		1	2	5	43
2011	2	1	11	5	4	1	1	4	7		1		6	43
2012	2		10	6	3	1		3	6				5	36
TOTAL	383	90	419	23	9	8	2	63	458	27	20	11	16	1529

FMFFaculty of Mathematics and Physics, University of LjubljanaFKKT (Uni-Lj)Faculty of Chemistry and Chemical Technology, University of LjubljanaFKKT (Uni-Mb)Faculty of Chemistry and Chemical Technology, University of MariborNTFFaculty of Natural Sciences and Engineering, University of LjubljanaFDVFaculty of Social Sciences, University of LjubljanaFAFaculty of Administration, University of LjubljanaBFBiotechnical Faculty, University of LjubljanaFEFaculty of Electrical Engineering, University of Ljubljana

Faculty of Computer and Information Science, University of Ljubljana Faculty of Civil Engineering, University of Maribor

 FERI
 Faculty of Electrical Engineering and Computer Science, University of Maribor

 UNG
 University of Nova Gorica

 IPS
 Jožef Stefan International Postgraduate School

 Other UNILJ
 Faculty of Pharmacy, Faculty of Mechanical Engineering, Faculty of

Economics, Faculty of Medicine, University of Ljubljana

FRI

FG

COMPLETED THESES

UNTIL 2012

Year	Ph. D.	M. Sc.	Total	Year	Ph. D.	M. Sc.	Total
	Theses	Theses			Theses	Theses	
1962	15	6	21	1988	12	26	38
1963	7		7	1989	15	33	48
1964	7	2	9	1990	16	41	57
1965	16		16	1991	22	47	69
1966	2		2	1992	19	42	61
1967		8	8	1993	28	36	64
1968	4	8	12	1994	27	37	64
1969	3	6	9	1995	34	22	56
1970	2	12	14	1996	38	25	63
1971	7	6	13	1997	29	23	52
1972	11	24	35	1998	21	20	41
1973	8	14	22	1999	33	29	62
1974	21	10	31	2000	36	27	63
1975	10	20	30	2001	31	28	59
1976	6	31	37	2002	29	19	48
1977	5	16	21	2003	41	19	60
1978	10	20	30	2004	31	20	51
1979	7	11	18	2005	22	7	29
1980	13	10	23	2006	22	2	24
1981	12	15	27	2007	26	7	33
1982	13	18	31	2008	29	5	34
1983	5	10	15	2009	30	7	37
1984	14	17	31	2010	33	5	38
1985	6	14	20	2011	31	2	33
1986	8	15	23	2012	47	4	51
1987	18	21	39	TOTAL	932	847	1779



PATENTS GRANTED

- Matthew Bogyo, Steven H. L. Verhelst, Marko Fonović Mild chemically cleavable linker system Patent No. US8314215 (B2), United States Patent and Trademark Office, 20.11.2012.
- Miran Mozetič, Alenka Vesel, Uroš Cvelbar Method and device for local functionalization of polymer materials Patent No. US8247039 (B2), United States Patent and Trademark Office, 21.8.2012.
- Luca Gregoratti, Marco Peloi, Marija Kosec, Danjela Kuščer A material in the form of lithium fluoride powder containing colour centres, method for preparation and use thereof Patent No. IT1397095, Notarbartolo & Gervasi S.P.A., 28.12.2012.
- Saša Novak, Nataša Drnovšek, Gregor Murn Bone implants with multilayered coating and process of their preparation Patent No. SI23420 (A), Slovenian Intellectual Property Office, 31.1.2012.
- Aleš Dakskobler, Andraž Kocjan, Manca Logar Method for the preparation of carrier colloidal powder with high specific surface area
 - Patent No. SI23502 (A), Slovenian Intellectual Property Office, 30.4.2012.
- Matjaž Panjan, Miha Čekada, Peter Panjan, Damjan Matelič, Andrej Mohar, Tomaž Sirnik, Jožko Fišer Hard protective coatings with the ability to change their color
 - Patent No. SI23538 (A), Slovenian Intellectual Property Office, 31.5.2012.
- Helena Razpotnik, Ivan Lavrač, Janez Holc, Danjela Kuščer, Marija Kosec Procedure for fabrication of alumina porcelain with improved mechanical properties
 - Patent No. SI23546 (A), Slovenian Intellectual Property Office, 31.5.2012. Igor Muševič, Matjaž Humar
- Spherical liquid crystal laser Patent No. SI23567 (A), Slovenian Intellectual Property Office, 31.5.2012.
- Aleš Dakskobler, Andraž Kocjan, Manca Logar Method for the preparation of carrier colloidal powder with high specific surface area
 - Patent No. SI23580 (A), Slovenian Intellectual Property Office, 26.6.2012.

- Aljaž Drnovšek, Dragan D. Mihailović An array smell sensor based on the measurement of the junction resistance of nanowires with different metals Patent No. SI23582 (A), Slovenian Intellectual Property Office, 29.6.2012.
- Marin Berovič, Darko Makovec, Suzana Bošković Process of magnetic precipitation of yeast biomass from sparkling wine Patent No. SI23583 (A), Slovenian Intellectual Property Office, 29.6.2012.
- Roman Novak, Matjaž Vencelj Method for quantum distribution of the short-range key Patent No. SI23596 (A), Slovenian Intellectual Property Office, 29.6.2012.
- Aljoša Maglica, Kristoffer Krnel, Tomaž Kosmač Single-stage process of manufacturing a composite ceramic heater Patent No. SI23609 (A), Slovenian Intellectual Property Office, 31.7.2012.
- Rok Zaplotnik, Alenka Vesel, Miran Mozetič Device for high-frequency gas plasma excitation Patent No. SI23611 (A), Slovenian Intellectual Property Office, 31.7.2012.
- Gregor Primc, Miran Mozetič Method for dynamically controlling the density of neutral atoms in a plasma vacuum chamber and a device for the processing of solid materials by using this

method Patent No. SI23626 (A), Slovenian Intellectual Property Office, 31.7.2012.

16. Janez Holc, Kostja Makarovič, Darko Belavič, Marko Hrovat, Marija Kosec, Boris Jordan

The manufacturing process of voids in the ceramic multi layered structures Patent No. SI23761 (A), Slovenian Intellectual Property Office, 31.12.2012.

- Lovro Gorjan, Aleš Dakskobler Sintering heat treatment procedure of formpieces Patent No. SI23763 (A), Slovenian Intellectual Property Office, 31.12.2012.
- Adolf Jesih, Andrej Kovič, Aleš Mrzel Method for a synthesis of quasi-one-dimensional structures of 4d and 5d (Nb, Mo Ta, W) transition metals Patent No. SI23768 (A), Slovenian Intellectual Property Office, 31.12.2012.

AWARDS AND APPOINTMENTS

AWARDS MADE TO JSI RESEARCHERS BY THE REPUBLIC OF SLOVENIA

Zois Award and Zois Certificate of Recognition

Janez Bonča

Presented with the Zois Award for the highest scientific achievements in the solid state theory of strongly correlated electron systems

Boštjan Golob, Samo Korpar, Marko Starič

Presented with the Zois Award for special achievements in particle physcis

Puh Certificate of Recognition

Damir Vrančić (JSI), Samo Krančan (Danfoss Trata, Ljubljana), Zoran Šaponia (Danfoss Trata, Ljubljana), Aleš Svetek (JSI), Ivan Kočar (Danfoss Trata, Ljubljana) Presented with the Puh Certificate of Recognition for the invention of intelligent motor drives for valves

JSI AWARDS AND APPOINTMENTS

The Jožef Stefan Golden Emblem Prize

presented to the following for doctoral theses with high impact :

Jernej Mravlje

The influence of phonons on electron transport in nanoscopic systems

Petra Brožič

Preparation of recombinant human hydroxysteroid dehydrogenases and study of their inhibitors

Andrej Gams Control of periodic and aperiodic robot movement using nonlinear oscillators

SELECTED OTHER AWARDS TO JSI RESEARCHERS

Jan Babič, Luka Peternel, Best Paper Student Award at a conference Robotics in Alpe-Adria-Danube Region 2012, Naples, Italy (awarded by the conference organizers)

Pavle Boškoski, Matej Gašperin, Dejan Petelin were the runners up in the IEEE PHM 2012 Prognostic Challenge (Data Challenge). They were invited to present their work at the 2012 IEEE International Conference on Prognostics and Health Management, Denver, Colorado, USA



The recipients of Zois awards and recognitions

Milan Brumen, "Srebrni znak Univerze v Mariboru" for successfull pedagogical and science research work at the University of Maribor

Raluca Camelia Frunza, best poster paper award TCM2012, TCM2012, Crete, Greece, October 26, 2012

Radojko Jaćimović, awarded the degree of Honorary Doctor by Odessa National Polytechnic University, Ukraine, 23. 10. 2012

Juš Kocijan, "Best paper award" during the conference Applied Mathematics, Simulation, Modelling 2012, North Atlantic University Union NAUN with paper Dynamic GP models: an overview and recent developments, Vougliameni, Greece

Anton Kokalj, Pregl Awards for Exceptional Achievements for Important Scientific Contribution in the Field of Chemistry and Associated Science

Primož Koželj, Prešern award of the Faculty of mathematics and Physics for Diploma thesis, University of Ljubljana, Ljubljana, Electrical, magnetic, and thermal properties of the δ -FeZn10 complex intermetallic phase

Samo Kralj, Golden sign, Maribor, University of Maribor

Urban Kuhar, First place on the student competition for article «The design of a low-cost beacon receiver based on software defined radio«, 21st International Electrotechnical and Computer Science Conference, Portorož, 18 September 2012

Martina Lorenzetti, Saša Novak, Spomenka Kobe, 2nd best oral presentation in Young researchers section, 20th Jubilee Conference on Materials and Technology, 17–19 October 2012, Portorož, Slovenia, given by the conference committee. Awarded contribution: Investigation of the properties of Titania coatings on Ti-based alloys substrates for body IMP.

Martina Modic, Award for the best Poster on 14th Joint Vacuum Conference, Poster with title "Shear stress and platelet adhesion on plasma treated polymer surfaces".

Jernej Mravlje, Prix de la Foundation Hugot du College de France, College de France, Paris, France

Nikola Novak, Best paper award, Ljubljana, 4th Student Conference of the Jožef Stefan International Postgraduate School, Jožef Stefan International Postgraduate School

Gregor Posnjak, Prešern award of the Faculty of mathematics and Physics for Diploma thesis, Ljubljana, University of Ljubljana, Magnetic structure determination of one-dimensional antiferromagnet CuSe205 with neutron scattering

Peter Rodič, Ingrid Milošev, Jernej Iskra, Barbara Kapun, Rector's Award for the third best innovation of University in Ljubljana, for the year 2012

Miha Škarabot, Igor Muševič, Luckhurst Samulski Prize, Mainz, Liquid Crystals

Tomaž Šolc, Award for the best paper for article "Spectrum Sensing for Cognitive Wireless Applications Inside Aircraft Cabins", 31st 2012 IEEE/AIAA Digital Avionics Systems Conference, Williamsburg, Virginia, USA, 14-18 October 2012

Uroš Tkalec, Glenn H. Brown Prize, Mainz, International Liquid Crystal Society

Aleš Ude, Award for the paper titled "Integrating surface-based hypotheses and manipulation for autonomous segmentation and learning of object representations", which was the finalist for the best-cognitive-paper award at the IEEE International Conference on Robotics and Automation (ICRA), held in St. Paul, MN, USA. ICRA is a prime conference in the area of robotics worldwide

Mihaela Uplaznik, Leon Cizelj and Igor Simonovski, The Best Poster Awards, International Conference Nuclear Energy for New Europe 2012, Ljubljana, "Cohesive Based Surface Approach for Grain Boundary Modelling"

Boris Žemva, Award for the Mentor of the Year 2012, given by young researches association of Slovenia.



The winners of the Jožef Stefan Golden Emblem Prize

REVIEW OF PUBLICATIONS

FOR 2012

Department	Original Articles*	Books	Patent Appl. and	Theses
			Grants	
Department of Theoretical Physics (F-1)	165			4
Department of Low and Medium Energy Physics (F-2)	62	1	1	2
Department of Thin Films and Surfaces (F-3)	22		2	1
Department of Surface Engineering and Optoelectronics (F-4)	80		5	3
Department of Solid State Physics (F-5)	150	2	2	6
Department for Complex Matter (F-7)	34	3	5	1
Department of Reactor Physics (F-8)	60			2
Department of Experimental Particle Physics (F-9)	215	3		2
Department of Inorganic Chemistry and Technology (K-1)	35		3	1
Department of Physical and Organic Chemistry (K-3)	25		1	1
Electronic Ceramics Department (K-5)	63	2	5	2
Engineering Ceramics Department (K-6)	16		5	2
Department for Nanostructured Materials (K-7)	68	2	2	2
Department for Synthesis of Materials (K-8)	36		1	2
Department for Advanced Materials (K-9)	45		4	2
Department of Biochemistry, Molecular and Structural Biology (B-1)	39	3	1	2
Department of Molecular and Biomedical sciences (B-2)	11	1		
Department of Biotechnology (B-3)	46	3	3	1
Department of Environmental Sciences (0-2)	129	16		2
Department of Automation, Biocybernetics and Robotics (E-1)	52		1	
Department of Systems and Control (E-2)	44			3
Artificial Intelligence Laboratory (E-3)	40	3		2
Laboratory for Open Systems and Networks (E-5)	22			
Department of Communication Systems (E-6)	62	3	1	
Computer Systems Department (E-7)	30	1		1
Department of Knowledge Technologies (E-8)	66	4		3
Department of Intelligent Systems (E-9)	75	1	3	2
Department of Reactor Engineering (R-4)	79	2		1
Reactor Infrastructure Centre (RIC)	40	2		
Centre for Networking Infrastructure (CNI)	2	1		
Energy Efficiency Centre (EEC)	16	2		1
Milan Čopič Nuclear Training Centre (ICJT)	3			
Radiation Protection Unit (SVPIS)	1			
Centre for Technology Transfer and Innovation (CTT)	2	1		1
Jožef Stefan Institute	1634	52	38	51

* Articles in Journals and Conference Proceedings, and Chapters in Books

KNOWLEDGE TRANSFER

The JSI pays a lot of attention to furthering its links with industry. In keeping with European aims and the objectives of the Slovenian government, the JSI organized several important meetings on the subject of cooperation with enterprises and

R & D PROJECT PARTNERS

- 1. Acies bio d.o.o., Ljubljana
- 2. Ames d.o.o., Brezovica pri Ljubljani
- 3. ARAO Agency for Radwaste Management, Ljubljana, Ljubljana
- 4. B2 d.o.o., Ljubljana
- 5. Bia separations, d.o.o., Ajdovščina
- 6. Biomed d.o.o., Ljubljana
- 7. Cinkarna Celje, Celje
- 8. Danfoss Trata, d.o.o., Ljubljana
- 9. Domel, d.o.o., Železniki
- 10. Ekliptik, d.o.o., Ljubljana
- 11. Gen energija, d.o.o., Krško
- 12. Gorenje gospodinjski aparati, d.d., Velenje
- 13. Inea, d.o.o., Ljubljana
- 14. Informa Echo, d.o.o., Ljubljana
- 15. Institute of Oncology, Ljubljana, Ljubljana
- 16. Intech les, d.o.o., Rakek
- 17. Iskratel, d.o.o., Kranj
- 18. Jožef Stefan International Postgraduate School, Ljubljana
- 19. JP vodovod-kanalizacija, d.o.o., Ljubljana
- 20. Knauf Insulation, d.o.o., Škofja Loka
- 21. Kolektor Group, d.o.o., Idrija

industry. In this way the JSI introduced a new method of cooperation, showing industry and the public that it is aware of its leading role, not only in research but also in the transfer of knowledge into practice.

- 22. Krško Nuclear Power Plant, Krško
- 23. Lek, d.d., Ljubljana
- 24. Luka Koper, d.d., Koper
- 25. Magneti Ljubljana, d.d., Ljubjana
- 26. Milan Vidmar Electric Power Research Institute, Ljubljana
- 27. Ministry of Infrastructure and Spatial Planning of the Republic of Slovenia, Ljubljana
- 28. Ministry of Agriculture and the Environment of the Republic of Slovenia, Ljubljana
- 29. Ministry of Defence of the Republic of Slovenia, Ljubljana
- 30. Ministry of Economic Development and Technology of the Republic of Slovenia, Ljubljana
- 31. Ministry of Health of the Republic of Slovenia, Ljubljana
- 32. Nela razvojni center, d.o.o., Železniki
- 33. Petrol, d.d., Ljubljana
- 34. Razvojni center eNeM Novi Materiali, d.o.o., Zagorje
- 35. RŽV, d.o.o., Gorenja vas
- 36. Splošna bolnišnica "dr. Franca Derganca", Šempeter pri Gorici
- 37. Telekom Slovenije, d.d., Ljubljana
- 38. Termoelektrarna Toplarna Ljubljana, d. o. o., Ljubljana
- 39. University of Ljubljana, Ljubljana
- 40. Varsi, d.o.o., Ljubljana
- 41. Zavod Bris, Ljubljana



INSTITUTE IN NUMBERS

2011-2012

COMPARISON OF REVENUES $({\bigstar} M)$



REVENUES FROM OTHER ACTIVITIES $({ { { { { { { { CM } } } } } } } })$



855.02 837.82 900 200 700 600 500 2011 2012 400300 161.42 162.9 100 Total Researchers Young Researchers

REVENUES FROM PUBLIC SERVICES (€M)



NUMBER OF PUBLICATIONS IN THE WEB OF SCIENCE



NUMBER OF CITATIONS IN THE WEB OF SCIENCE



EMPLOYEES (FTE)

RESEARCH DEPARTMENTS

DEPARTMENT OF THEORETICAL PHYSICS F-1

The group of THEORETICAL PHYSICS OF NUCLEI, PARTICLES AND FIELDS has investigated the structure of hadrons, the effective theories of weak and electromagnetic mesonic decays, the unified theory of elementary interactions, the relativistic theory of membranes and precise calculations of the properties of three-body systems in atomic physics.

We performed the first lattice QCD simulation of the scattering between pion and kaon in the channels where the scalar and vector resonances have been observed. The calculated energy eigenstates qualitatively agree with the observed spectrum of resonances, while the calculated scattering phase shifts qualitatively agree with the measured ones. We derived the analytic relation between the energy levels on the lattice and the scattering phase shifts for the case of scattering between two particles with different masses and a non-zero total momentum.

We studied the top-quark substructure in electromagnetic weak and strong interactions. We explored the implications of the recent experimental evidence for charm CP violation. We then demonstrated the universality of CP Violation in Delta F = 1 processes. We also explored CP violation in the charm system via D to V gamma decays. We Head: studied the effects of hypothetical light neutral particles in decays of kaons, B mesons and the recently discovered Prof. Svjetlana Fajfer Higgs boson. We also studied minimal flavour-violating realisations of the see-saw mechanism of neutrino mass generation.

We have calculated cross-sections, forward-backward asymmetry and charge asymmetries for the production process of top and anti-top at Tevatropn and LHC. A number of top-spin observables have been considered, which might help in constraining models of New Physics.

We show that the charge asymmetry in t tbar production at the LHC, and the forward-backward asymmetry at the Tevatron, are in general not tightly correlated. We demonstrate this using two examples of NP: a light axigluon, and a vector that is a colour octet and electroweak triplet. The small value of the charge asymmetry, measured at the LHC is thus shown not to exclude a NP interpretation of the anomalously large forward-backward asymmetry at the Tevatron.

We have classified scalar leptoquarks that destabilize the proton and pointed out the relevant higher order contributions of states, previously regarded as innocuous with respect to proton decay. We have proposed a combined analysis of the decays B -> K l+ l- and Bs -> l+ l- that could help determine complex phases of the Wilson coefficients. Furthermore, we have analysed the impact of all possible leptoquark scenarios in these decay modes.

Recently, the observed anomaly in B -> D* tau nu and B -> D tau nu has been investigated and we have found that by introducing most general scalar or tensor operators one can explain the experimental results. At the same time we have questioned the lepton flavour universality in these processes.

We have demonstrated how the recently emerged puzzle in the decay B -> D tau nu can be solved by introducing scalar or tensor effective operators. A new observable, defined on the phi resonance, has been put forward to search for direct CP violation in $D \rightarrow pi l+$ I- and Ds -> K I+ I- and independently test recent positive measurements of CP violation in D -> pi pi and D -> K K.

We showed it is possible to include direct CP violation in charm decays into the extraction of the weak phase of the standard model of elementary particles. We showed that the LHC does not exclude the anomalies in the production of top-antitop quark pairs. We showed that large flavour-violating branching ratios in the Higgs boson decay are possible. After the discovery of the Higgs boson we explored its significance for the solutions of the hierarchy problem. We derived astrophysics independent bounds on the annual modulation signal in direct dark matter detection.

Within the SU(5) unification theory we have investigated the role of coloured scalars in the processes of Higgs boson decay to two photons and we have found that a scalar octet or sextet can explain the observed difference of the measured decay width and the Standard Model Prediction.

At a 1-loop level we spontaneously broke both the supersymmetry and gauge symmetry of a unified SU(5). We showed that a scalar propagator at the boundary of AdS has a Goldstone pole due to the breaking of dilatation symmetry. Adding a pair of fundamental representations in a unified SU(5) we corrected the fermion mass relations increasing the proton lifetime.

We explored the implications of the recent experimental evidence for charm CP violation. A new observable, defined on the phi resonance, has been put forward to search for direct CP violation in D -> \pi I+ I- and D_s -> K I+ I- and independently test recent positive measurements of CP violation in D -> pi pi and D -> K K. We performed the first lattice simulation of the scattering between the pion and kaon in the resonant channels.







$\tilde{\mu}_t m_t$

Figure 1: Combined LHC (total (σ LHC) and differential (σ h,LHC) cross-sections are shown shaded) and Tevatron (shown in contours) constraints on the top quark chromomagnetic (μ t) and chromoelectric (dt) dipole moments. Indirect neutron electric dipole moment (nEDM) constraint on dt is shown in green.

We reviewed different phenomenological aspects of the seesaw mechanism for neutrino masses with electroweak triplets, in particular those related to the mass splitting of different components. We show an example of setting the limit from the LHC data, performed electroweak precision tests and studied the impact on the Higgs decay rate. We present a comprehensive analysis of the possibility to accommodate dark matter in the minimal left-right symmetric model at a low scale, accessible to the LHC. A detailed analytical and numerical study reveals the existence of a window for the right-handed gauge boson, accessible at the collider operating at an energy of 14 TeV.

We investigated the significance of orthogonal and symplecitc Clifford algebras in the quantization of point particles and fields. We have found that the generators of Clifford algebras have the role of quantum mechanical or quantum field operators and that they satisfy the Heisenberg equations of motion. We have also studied the Wheeler-DeWitt equation in five dimensions and showed that it contains the modified QED in the presence of gravity.

Using a purely numerical trick, regularization by error majorization, in the framework of the Quasilinearization Method, uniform stability and precision (up to 28 decimal places) was achieved for small and large couplings in

very singular potentials. This method covers more parameter space than any mixed perturbative/numerical method applied to the problem in the last couple of decades.

Some outstanding publications in the past year

- Isidori, G., Kamenik, J., Ligeti, Z., Perez, G.: Implications of the LHCb evidence for charm CP violation. Phys. lett., Sect. B. [Print ed.], 2012, vol. 711, no. 1.
- Fajfer, S. Kamenik, J., Nišandžić, I.: B[to] D[sup][ast][tau][nu][bar][sub][tau] sensitivity to new physics. Phys. rev., D Part. fields gravit. cosmol., 2012, vol. 85, no. 9, pp. 094025-1-094025-9.

In the group for THEORY OF CONDENSED MATTER AND STATISTICAL PHYSICS we investigated the properties of solids with strongly correlated electrons, superconductors, nanosystems, ferroelectrics and the behaviour of complex systems.

Within the theory of the out-of-equilibrium phenomena we continued our investigation of the behaviour of different model systems in the presence of an electric field. We performed an accurate time-dependent numerical

We performed a time-dependent numerical analysis of the response of a two-hole bound state in the t-J model. We showed that the decay of the bound state coincides with the onset of a finite steady current in the case where the degrees of freedom of a binding mechanism and of energy dissipation are the same. study of an out-of-equilibrium response of a two-hole bound state within a t-J model. We show that a bound hole pair decays with the onset of a finite steady current if both mechanisms for binding and dissipation share matching degrees of freedom. Keeping the full quantum nature of the problem, we calculated the relaxation time of the Holstein polaron in one dimension after it was driven far out of equilibrium by a strong electromagnetic pulse. The dynamics of the relaxation is seen as a decrease of the kinetic energy at the expense of increased elastic energy due to the excitation of phonons. We studied the breakdown of a Mott insulator due to the external electric

field. We showed that the probability for the breakdown can be calculated analytically and that it deviates from the estimates obtained by approximate calculations.

In connection with the broader investigation of correlated systems we continued the analysis of the behaviour of spin-chain models. We showed that the anisotropic Heisenberg model has anomalous behaviour in the hydrodynamic regime of small wave-vectors and low frequencies. We showed that the model exhibits the coexistence of normal spin diffusion and anomalous behaviour of an ideal insulator in the insulating regime at high temperatures. With co-workers we investigated quasi-particle properties of the correlated materials with high electrical resistivity, and the optical response of the Fermi liquids. We also collaborated on a review article about Hund's rule coupling in correlated metals. Within the research of superconductors, we described with the model self-energy the transport properties like resistivity, optical conductivity and Hall coefficient in a normal phase of overdoped cuprates. In collaboration with experimental groups we extended the theory of electro-calorical phenomena in relaxor ferroelectrics for cases of ferroelectric polymers. Within the spherical random field - random bond model of relaxors we additionally treated the coupling between dielectric polarization and lattice deformations.

Within the theory of nanosystems we studied the properties of double quantum dot systems with unusual ground states. We proved that the system of two parallel quantum dots has a ground state, which is a singular Fermi liquid. We showed that in the system of two serial quantum dots with ferromagnetic leads one can control the direction of the spin current using electrostatic potentials. For a system of three capacitatively coupled quantum dots we observed that by increasing the ratio between interdot and intradot repulsion there is a collective Kondo effect.

Within the research in the field of statistical physics of complex systems and networks we studied empirical data on the communications between users of social networks and those of the world wide web. On the basis of collected information on dynamics and the emotional content of all the dialogs we determined the statistical laws of the spreading of emotions between MySpace users. We also studied the networks that emerge on the basis of the self-organizing dynamics of random communications of a particular content, and showed that these networks are hierarchically organized.

Some outstanding publications in the past year



Figure 2: The colour map represents the quasiparticle weight, with the bright colours corresponding, as a function of the filling and interaction strength in the 3-orbital Hubbard model with semicircular density of states. Black vertical bars indicate the Mott insulating state. The key to the qualitatively different behaviour at different electronic occupation is the Hund's rule coupling.

- Žitko, R., Mravlje, J., Haule, K.: Ground state of the parallel double quantum dot system. Phys. rev. lett., 2012, 1. vol. 108, no. 6, pp. 066602-1-066602-5.
- Lenarčič, Z., Prelovšek, P.: Dielectric breakdown in spin-polarized Mott insulator. Phys.rev. lett., 2012, vol. 108, 2. iss. 19, pp. 196401-1-196401-4.

The group of THEORETICAL BIOPHYSICS AND SOFT MATTER PHYSICS investigated polyelectrolytes, liquid crystals, colloids, and phospholipid and biological membranes

We analysed some aspects of physical virology, especially the contribution of electrostatic interactions to the stability of viral capsids. By carrying out a detailed statistical analysis of structural characteristics of viruses, we

delineated the properties of models that can be used to describe them. Using molecular dynamics simulations we investigated the properties of biological membranes, focusing on the hydration repulsion between them. We studied the interaction between two neutral dielectric bodies in the presence of a highly asymmetric ionic fluid containing multivalent as well as monovalent salt ions. We derived the correct coarse-grained model of the interactions between colloids coated with short DNA

segments. We studied the phase behaviour of hard-sphere colloids confined in a harmonic potential.

We developed a methodology for the analysis of three-dimensional confocal microscope images of lipid vesicles and we used it to study the spontaneous transformations of vesicles. We quantified the main morphometric param-

eters of a broad range of axisymmetric and non-axisymmetric shapes and we showed that both the stable and the transient shapes can be described in terms of the theory of elasticity. The experimentally observed shapes were arranged in the phase diagram. Also studied was the dynamics of adhesion of liposomes on a charged electrode. We proposed a mechanical model of liposome deformation during the process. By analysing the amperometric signals, we found that upon adhesion, the water content of the liposome is released through the pores formed in the membrane.

Using a two-dimensional mechanical model, we theoretically studied gastrulation in the fruit fly which begins with the formation of ventral furrow. We showed that the furrow formation can be attributed to an elastic instability of the embryonic epithelium sandwiched between the vitelline membrane and the yolk. Within our model, the only role of cell differentiation is to pin the furrow at a predetermined location. This can be achieved by a slightly increased size of mesoderm cells, which is consistent with experimental observations.

We studied the dependence of the behaviour of phospholipid vesicles on the presence of substances that form membrane pores. It was shown that Figure 3: Reconstructed 3D confocal-microscope images of lipid vesicles polyen nistatin forms pores even in sterol-free membranes. A model was (graphics A. Šiber)

Using a new model of erythrocyte spectrin skeleton, we analysed the dependence of a cell 's deformability on its stress-free state.

introduced to describe the dynamic changes of membrane permeability caused by the component of the bee venom melittin. We discussed the properties of lipid vesicles that may have given rise to cellular life. Using a new model of erythrocyte spectrin skeleton, we analysed the dependence of the cell's deformability on its stress-free state.

The mathematical model of arachidonic acid metabolism influenced by the addition of aspirin and related anti-rheumatic drugs was extended and adapted for use in the clinical treatment of asthmatic patients intolerant to these medications. We theoretically predicted several scenarios of avoiding asthma symptoms after anti-rheumatic drugs were administered. We have explored different regimes of coarse-grained modelling of bacterial chemotaxis, identifying regions in parameter space where Weber logarithmic law applies and regions where sensing depends on the absolute concentration gradients.

We analysed an old problem of the dynamics of ferroelectric liquid crystals close to the phase transition and we showed that they are characterized by four and two modes below and above the transition, respectively. Upon increasing and decreasing the temperature away from the phase transition, the predominantly tilt or polar character of the modes is lost and the frequency of the mode is no longer a linear function of temperature.

Also studied were the optical properties of ferrofluid dispersions of cobalt nanoparticles in cyclohexane, which can be modified significantly by weak magnetic fields. We studied the induced linear birefringence and the optical activity as a function of nanoparticle size, their volume concentration, wavelength of light, and magnetic field strength.

Some outstanding publications in the past year

- Badasyan A., Tonoyan, Sh. A., Giacometti, A., Podgornik, R., Parsegian, V. A., Mamasakhlisov, Y. S., Morozov, V.: Osmotic pressure induced coupling between cooperativity and stability of a helix-coil transition. Phys. rev. lett., 2012, vol. 109, iss. 6, pp. 068101-1-068101-5.
- Hočevar Brezavšček, A., Rauzzi, M., Leptin, M., Ziherl, P.: A model of epithelial invagination driven by collective mechanics of identical cells. Biophys. j., 2012, vol. 103, no. 5, pp. 1069-1077.

Organization of conferences, congresses and meetings

- 1. LOTHERM Summer School: Dynamics and Transport in Quantum Magnets, Ljubljana, 4.-6. 6. 2012
- 2. Hadronic Resonance, Bled, 1.-8. 7. 2012
- 3. Mechanics of Tissues, Ljubljana, 29.-30. 10. 2012

Awards and appointments

- 1. Prof. Janez Bonča: Zois award for the highest scientific achievements: Research in the solid state theory of strongly correlated electron systems
- 2. Dr. Jernej Mravlje: Zlati znak Jožef Stefan: The influence of phonons on electron transport in nanoscopic systems
- 3. Dr. Jernej Mravlje: Prix de la Foundation Hugot du College de France, College de France, Paris, France,
- 4. Prof. Milan Brumen: "Srebrni znak Univerze v Mariboru" for successfully pedagogical and science research work at the University of Maribor

INTERNATIONAL PROJECTS

- Mechanics of Tissues workshop, Ljubljana, 29.–30.10.2012 European Science Foundation Prof. Primož Ziherl
- 7. FP . Cyberemotions: Collective emotions in cyberspace European Commission
- Prof. Bosiljka Tadić 3. 7. FP - LOTHERM: Low dimensio
- 7. FP LOTHERM: Low dimensional quantum magnets for thermal management European Commission Prof. Peter Prelovšek
- 7. FP COMPLOIDS: Physics of complex colloids: Equilibrium and driven European Commission
- Prof. Primož Ziherl 5. Self-assembly in ionic liquids
- University College London Prof. Rudolf Podgornik
- Scientific Meeting "The Role of Heavy Fermions in Fundamental Physics", Portorož, Slovenia, 11.–14. 4. 2011 Prof. Svietlana Faifer
- COST TD1210: Analysing the dynamics of information and knowledge landscapes Cost Office
 Cost Office
 - Prof. Bosiljka Tadić

- Supersymmetry and grand unification Slovenian Research Agency Prof. Borut Bajc
- Correlated electron systems coupled to lattice degrees of freedom Slovenian Research Agency Prof. Janez Bonča
- Interplay between precision measurements and LHC discoveries Slovenian Research Agency
- Asst. Prof. Jernej Fesel Kamenik 11. Theoretical studies of dynamical properties in correlated electron systems coupled to
 - external degrees of freedom Slovenian Research Agency
- Prof. Janez Bonča
- Flavor violation at the Large Hadron Collider Slovenian Research Agency Asst. Prof. Jernej Fesel Kamenik
- Aspects of the AdS-CFT correspondence in particle physics and cosmology Slovenian Research Agency Prof. Borut Baic

RESEARCH PROGRAMS

- Theory of the condensed matter and statistical physics 1. Prof. Janez Bonča
- 2. Theoretical physics of nuclei, particles and fields Prof. Svjetlana Fajfer
- Biophysics of polymers, membranes, gels, colloids and cells 3 Prof. Rudolf Podgornik

R & D GRANTS AND CONTRACTS

1. Theoretical aspects and empirical analysis of labour market impact of flexicurity Dr. Jernej Mravlje

VISITORS FROM ABROAD

- 1. Prof. Joachim Brod, Technische Universität, Munich, Germany, 4.-7. 1. 2012
- Dr. Elaine Fortes, Instituto de Física Teórica, Sao Paulo, Brazil, 19.-21. 1. 2012 2.
- 3. Prof. Blaženka Melić, Institut Ruđer Bošković, Zagreb, Croatia, 23.-24. 1. 2012
- Prof. John H. Jefferson, Oxford University, Oxford, Great Britain, 23.-28. 1. 2012
- Dr. Tirtha Sankar Ray, Institut de Physique Théorique, CEA Saclay, Saclay, France, 5. 24.-27. 1. 2012
- 6. Dr. Michele Frigerio, Universite Montpellier, Montpellier, France, 27. 1.-1. 2. 2012 Dr. Takshi Toma, Institute for Theoretical Physics, Kanazawa University, Kanazawa,
- Japan, 8,-12, 2, 2012 Prof. Stefan Thurner, Complex Systems Research Group, Medical University of Vienna, 8. Vienna, Austria, 16.–18. 2. 2012
- Prof. Marcin Mierzejewski, University of Katowice, Katowice, Poland, 12.-18. 2. 2012, 28. 10.-18. 11. 2012
- 10. Dr. Adriano Amaricci, CNR-Instituto Officina dei Materiali Internationa School for Advance Studies, Trieste, Italy, 20. 3. 2012
- 11. Dr. Sogee Spinner, SISSA-Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy, 22.-24. 3. 2012
- 12. Prof. Adriano Lugo, Universidad Nacional de La Plata, La Plata, Argentina, 2.–14. 4. and 30.7.-13.8.2012
- 13. Dr. Sebastien Descotes Genon, Laboratorie de Physique Theorique, CNRS, Paris, France, 9.-16.5., 22.-27.11.2012
- 14. Prof. Thomas Mannel, Universität Siegen, Siegen, Germany, 18.-23. 5. 2012
- 15. Dr. Benoit Blossier, Universite Paris Sud, Paris, France, 23.-28. 5. 2012

STAFF

Researchers

- Prof. Borut Bajc 1.
- 2. Prof. Janez Bonča*
- Prof. Milan Brumen* 3.
- Prof. Mojca Čepič* 4.
- Prof. Jure Dobnikar 5.
- 6. Prof. Svjetlana Fajfer*, Head
- Asst. Prof. Jernej Fesel Kamenik 7.
- Prof. Bojan Golli* 8
- Dr Raimund Krivec 9
- 10. Dr. Miha Nemevšek
- 11. Dr. Matej Pavšič, retired 28.07.12
- Prof. Raša Matija Pirc, retired 28.07.12
 Prof. Rudolf Podgornik*
- Prof. Peter Prelovšek*
- 15. Asst. Prof. Saša Prelovšek Komelj*
- 16. Prof. Anton Ramšak*
- 17. Dr. Tomaž Rejec*
- 18. Dr. Igor Sega
- 19. Dr. Robin Steinigeweg, left 01.08.12
- 20. Prof. Saša Svetina
- 21. Dr. Milovan Šuvakov 22. Prof. Bosiljka Tadić
- 23. Prof. Nataša Vaupotič* 24. Asst. Prof. Darko Veberič*
- 25. Prof. Primož Ziherl*
- 26. Asst. Prof. Jure Zupan
- 27. Dr. Rok Žitko

Postdoctorial associates

28. Dr. Artem Badasyan, left 01.11.12 29. Dr. Jure Drobnak

- 2 Theory of thermal and spin transport in novel materials with correlated electrons Prof Peter Prelovšek
- 3. Superconductivity and magnetism in new iron-based superconductors Prof. Peter Prelovšek
- Non-equilibrium dynamics of interacting electron systems
- Prof. Peter Prelovšek 5. Hadronic resonances
- Prof. Bojan Golli
- 6. Synergies between precision measurements and LHC discoveries Asst. Prof. Jernej Fesel Kamenik
- Theory of materials for spin electronics and dynamics of magnetic nanostructures Prof. Janez Bonča
- 8. LdV: Training in the frame of the Leonardo da Vinci mobility at the Foreign Institute -ISIT
- Dr. Miha Nemevšek
- 16. Prof. Ilja Doršner, Univerza v Sarajevu, Sarajevo, Bosnia and Herzegovina, 29. 5.-3. 6. 2012, 11. 7.-15. 8. 2012, 3.-10. 11. 2012
- 17 Prof. Vikram Soni, National Physical Laboratory and Jamia Millia University, New Delhi, India, 17. 6.-1. 7. 2012
- 18. Dr. Greg M. Grason, University of Massachusetts, Amherst, USA, 14.-31. 7. 2012
- 19. Prof. Masayuki Imai, Ochanomizu University, Tokyo, Japan, 16.-19. 7. 2012
- 20. Prof. C. S. Kim, Department of Physics and IPAP, Yonsei University, Seoul, Korea, 24.-27. 8.2012
- 21. Prof. Thomas Pruschke, Institute for Theoretical Physics, Gottingen, Germany. 26.-30.8.2012
- 22. Prof. Paul Loosdrecht, University of Groningen, Groningen, Netherlands, 9.-11. 9. 2012
- 23. Prof. Yoshikazu Fujiwara, University of Kyoto, Kyoto, Japan, 19.-23. 9. 2012
- 24. Prof. Murugappan Muthukumar, Department of Polymer Science and Engineering,
- University of Massachusetts, Amherst, USA, 19.-23. 9. 2012
- 25. Dr. Charanjit S. Aulakh, Department of Physics, Panjab University, Chandigarh, India, 24.-28.9.2012
- 26. Dr. Krzysztof Bieniasz, M. Smoluchowski Institute of Physics, Jagellonian University, Krakow, Poland, 3.-10. 11. 2012
- Dr. Maria Vittoria Garzelli, univerza v Novi Gorici, Nova Gorica, Slovenia, 8. 11. 2012 27
- 28. Dr. Antonio Šiber, Institut za fiziku, Zagreb, Croatia, 19.-30. 11. 2012
- 29. Dr. Estefania Coluccio Leskow, Universidad de Buenos Aires, Buenos Aires, Argentina, 21. 11.-21. 12. 2012

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- 30. Dr. Ana Hočevar Brezavšček
- 31. Dr. Julio Julio
- 32. Dr. Matej Kanduč
- 33. Dr. Jure Kokalj
- 34. Dr. Nejc Košnik
- 35. Dr. Jernej Mravlje
- 36. Dr. Luca Tubiana
- 37. Dr. Lev Vidmar

38. Dr. Mihael-Matjaž Zemljič*

Postgraduates

- 39. Lamprini Athanasopoulou, B. Sc.
- 40. Denis Golež, B. Sc.
- 41. Admir Greljo, B. Sc.
- Jacek Wojciech Herbrych, M. Sc.
 Tilen Huljev Čadež, B. Sc.
- 44. Urška Jelerčič, B. Sc.
- 45. Jan Kogoj, B. Sc.
- 46. Ambrož Kregar, B. Sc.
- 47. Zala Lenarčič, B. Sc.
- 48. Luka Leskovec, B. Sc.

53. Žiga Osolin, B. Sc.

54. Vasja Susič, B. Sc.

55. Nevenka Hauschild

* part-time JSI member

Note:

Annual Report 2012

- 49. Anže Lošdorfer Božič, B. Sc.
- 50. Timon Mede, B. Sc.
- 51. Marija Mitrović, M. Sc., left 01.04.12 52. Ivan Nišandžić, B. Sc.

Technical and administrative staff

BIBLIOGRAPHY

ORIGINAL SCIENTIFIC ARTICLE

- 1. NA61/SHINE Collaboration: N. Abgrall *et al.* (137 authors), "Measurement of production properties of positively charged kaons in proton-carbon interactions at 31 GeV/c", *Phys. rev. C. Nucl. phys.*, vol. 85, no. 3, pp. 035210-1-035210-10, 2012.
- AUGER Collaboration: P. Abreu *et al.* (496 authors), "Description of atmospheric conditions at the Pierre Auger Observatory using the Global Data Assimilation System (GDAS)", *Astropart. phys.*, vol. 35, no. 9, pp. 591-607, 2012.
- 3. AUGER Collaboration: P. Abreu *et al.* (499 authors), "Measurement of the proton-air cross section at $\sqrt{s} = 57$ TeV with the Pierre Auger Observatory", *Phys. rev. lett.*, vol. 109, no. 6, pp. 062002-1-062002-9, 2012.
- 4. AUGER Collaboration: P. Abreu *et al.* (511 authors), "The rapid atmospheric monitoring system of the Pierre Auger Observatory", *Journal of instrumentation*, vol. 7, no. 9, pp. P09001-1-P09001-40, 2012.
- AUGER Collaboration: P. Abreu *et al.* (500 authors), "A search for anisotropy in the arrival directions of ultra high energy cosmic rays recorded at the Pierre Auger Observatory", *Journal of cosmology and astroparticle physics*, vol. 2012, no. 4, art. no. 40, 14 pp., apr. 2012.
 AUGER Collaboration: P. Abreu *et al.* (518 authors), "Search for point-
- AUGER Collaboration: P. Abreu *et al.* (518 authors), "Search for pointlike sources of ultra-high energy neutrinos at the Pierre Auger Observatory and improved limit on the diffuse flux of tau neutrinos", *The astrophysical journal, Letters*, vol. 755, no. 1, pp. L4-1-L4-7, 2012.
- 7. AUGER Collaboration: P. Abreu *et al.* (498 authors), "Search for signatures of magnetically-induced alignment in the arrival directions measured by the Pierre Auger Observatory", *Astropart. phys.*, vol. 35, no. 6, pp. 354-361, 2012.
- AUGER Collaboration: P. Abreu *et al.* (493 authors), "Erratum to "The Lateral Trigger Probability function for the Ultra-High Energy Cosmic Ray Showers detected by the Pierre Auger Observatory" [Astroparticle Physics 35 (2011) 266-276]", *Astropart. phys.*, vol. 35, no. 10, pp. 681-684, 2012.
- 9. AUGER Collaboration: P. Abreu *et al.* (515 authors), "Antennas for the detection of radio emission pulses from cosmic-ray induced air showers at the Pierre Auger Observatory", *Journal of instrumentation*, vol. 7, no. 10, pp. P10011-1-P10011-42, 2012.
- AUGER Collaboration: P. Abreu *et al.* (513 authors), "Large-scale distribution of arrival directions of cosmic rays detected above 10¹8 eV at the Pierre Auger Observatory", *Astrophys. J., Suppl. Ser.*, vol. 203, no. 2, pp. 34-1-34-20, 2012.
- 11. AUGER Collaboration: P. Abreu *et al.* (512 authors), "Results of a self-triggered prototype system for radio-detection of extensive air showers at the Pierre Auger Observatory", *Journal of instrumentation*, vol. 7, no. 11, pp. P11023-1-P11023-28, 2012.
- 12. AUGER Collaboration: P. Abreu *et al.* (509 authors), "A search for point sources of EeV neutrons", *Astrophys. J.*, vol. 760, no. 2, pp. 1-11, 2012.
- 13. AUGER Collaboration: R. Bonino *et al.* (479 authors), "Large scale anisotropy studies with the Pierre Auger Observatory", In: 3rd Roma International Conference on Astroparticle Physics (RICAP'11), May 25th - 27th, 2011 - Roma, Italy, *Nuclear instruments and methods in physics research, Section A, Accelerators, spectrometers, detectors and associated equipment*, vol. 692, pp. 88-92, 2012.
- 14. AUGER Collaboration: J. Chirinos *et al.* (510 authors), "Ground-truthing a satellite-based night-time cloud identification technique at the Pierre Auger Observatory", In: Focus point on interdisciplinary science with cosmic rays, *The European physical journal plus*, vol. 127, no. 8, pp. 1-10, 2012.
- AUGER Collaboration: S. Dasso *et al.* (483 authors), "The scaler mode in the Pierre Auger Observatory to study heliospheric modulation of cosmic rays", In: Advances in theory and observation of solar system dynamics I, *Advances in space research*, vol. 49, no. 11, pp. 1563-1569, 2012.
- 16. AUGER Collaboration: Benjamin Fuchs et al. (495 authors), "The Auger engineering radio array", In: 3rd Roma International Conference on Astroparticle Physics (RICAP'11), May 25th - 27th, 2011 - Roma, Italy, Nuclear instruments and methods in physics research, Section A, Accelerators, spectrometers, detectors and associated equipment, vol. 692, pp. 93-97, 2012.
- 17. AUGER Collaboration: Bianca Keilhauer *et al.* (510 authors), "Description of atmospheric conditions at the Pierre Auger

Observatory using meteorological measurements and models", In: Focus point on interdisciplinary science with cosmic rays, *The European physical journal plus*, vol. 127, no. 8, pp. 1-10, 2012.

- AUGER Collaboration: Karim Louedec *et al.* (510 authors), "Atmospheric aerosols at the Pierre Auger Observatory and environmental implications", In: Focus point on interdisciplinary science with cosmic rays, *The European physical journal plus*, vol. 127, no. 8, pp. 1-16, 2012.
- 19. AUGER Collaboration: R. Mussa *et al.* (510 authors), "Observation of ELVES at the Pierre Auger Observatory", In: Focus point on interdisciplinary science with cosmic rays, *The European physical journal plus*, vol. 127, no. 8, pp. 1-6, 2012.
- 20. AUGER Collaboration: Roberto Pesce *et al.* (504 authors), "Measuring the spectrum of UHECR with the Pierre Auger Observatory", In: 3rd Roma International Conference on Astroparticle Physics (RICAP'11), May 25th 27th, 2011 Roma, Italy, *Nuclear instruments and methods in physics research, Section A, Accelerators, spectrometers, detectors and associated equipment*, vol. 692, pp. 83-87, 2012.
- 21. AUGER Collaboration: V. Rizi *et al.* (510 authors), "Atmospheric monitoring with LIDARs at the Pierre Auger Observatory", In: Focus point on interdisciplinary science with cosmic rays, *The European physical journal plus*, vol. 127, no. 8, pp. 1-12, 2012.
- 22. AUGER Collaboration: Mariangela Settimo *et al.* (513 authors), "Measurement of the cosmic ray energy spectrum using hybrid events of the Pierre Auger Observatory", In: Focus point on interdisciplinary science with cosmic rays, The European physical journal plus, vol. 127, no. 8, vol. 127, no. 8, pp. 1-15, 2012.
- 23. AUGER Collaboration: L. Wiencke *et al.* (510 authors), "The Pierre Auger Observatory and interdisciplinary science", In: Focus point on interdisciplinary science with cosmic rays, *The European physical journal plus*, vol. 127, no. 8, pp. 1-7, 2012.
- 24. Dejan Arzenšek, Drago Kuzman, Rudolf Podgornik, "Colloidal interactions between monoclonal antibodies in aqueous solutions", *J. colloid interface sci.*, vol. 384, iss. 1, pp. 207-216, 2012.
- 25. K. S. Babu, Borut Bajc, Z. Tavartkiladze, "Realistic fermion masses and nucleon decay rates in supersymmetric SU(5) with vectorlike matter", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 86, no. 7, pp. 075005-1-075005-11, 2012.
- 26. Artem Badasyan A., Sh. A. Tonoyan, Achille Giacometti, Rudolf Podgornik, Vozken Adrian Parsegian, Yevgeni S. Mamasakhlisov, Vladimir Morozov, "Osmotic pressure induced coupling between cooperativity and stability of a helix-coil transition", *Phys. rev. lett.*, vol. 109, iss. 6, pp. 068101-1-068101-5, 2012.
- 27. Borut Bajc, Stéphane Lavignac, Timon Mede, "Supersymmetry breaking induced by radiative corrections", *J. high energy phys.*, vol. 2012, no. 7, pp. 185-1-185-17, 2012.
- 28. Borut Bajc, Adrián Lugo, Mauricio B. Sturla, "Spontaneous breaking of a discrete symmetry and holography", *J. high energy phys.*, vol. 2012, no. 4, pp. 119-1-119-19, 2012.
- 29. Damir Bečirević, Nejc Košnik, Federico Mescia, Ella Schneider, "Complementarity of the constraints on new physics from $B_s \rightarrow \mu^+\mu^$ and from $B \rightarrow Kl^+l^-$ decays", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 86, no. 3, pp. 034034-1-034034-15, 2012.
- 30. Damir Bečirević, Nejc Košnik, Andrey Tayduganov, " $\overline{B} \rightarrow D\tau \overline{n} u_{\tau}$ vs. $\overline{B} \rightarrow D\mu \overline{v_{\mu}}$ ", *Phys. lett., Sect. B*, vol. 716, no. 1, pp. 208-213, 2012.
- 31. AUGER Collaboration: C. Berat *et al.* (504 authors), "Radio detection of extensive air showers at the Pierre Auger Observatory", *Nucl. instrum, methods phys res., Sect. A, Accel.*, pp. 1-4, 2012.
- 32. Klemen Bohinc, Ahis Shrestha, Milan Brumen, Sylvio May, "Poisson-Helmholtz-Boltzmann model of the electric double layer: analysis of monovalent ionic mixtures", *Phys. rev., E Stat. nonlinear soft matter phys. (Print)*, vol. 85, no. 3, pp. 031130-1-031130-12, 2012.
- 33. Janez Bonča, Marcin Mierzejewski, Lev Vidmar, "Nonequilibrium propagation and decay of a bound pair in driven t-J models", *Phys. rev. lett.*, vol. 109, iss. 15, pp. 156404-1-156404-5, 2012.
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- 37. NA61/SHINE Collaboration: T. Cetner *et al.* (139 authors), "Methods to study event-by-event fluctuations in the NA61/SHINE experiment at the CERN SPS", *Phys. at. nucl.*, vol. 75, no. 5, pp. 567-570, 2012.
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- Ilja Doršner, Svjetlana Fajfer, Admir Greljo, Jernej Kamenik, "Higgs uncovering light scalar remnants of high scale matter unification", J. high energy phys., issue 11, vol. 2012, pp. 130-1-130-17, 2012.
- 51. Ilja Doršner, Svjetlana Fajfer, Nejc Košnik, "Heavy and light scalar leptoquarks in proton decay", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 86, no. 1, pp. 015013-1-015013-14, 2012.
- 52. Jure Drobnak, Alexander L. Kagan, Jernej Kamenik, Gilad Perez, Jure Zupan, "Forward Tevatron top quarks and backward LHC top quarks with associates", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 86, no. 9, pp. 094040-1-094040-13, 2012.
- Jure Drobnak, Jernej Kamenik, Jure Zupan, "Flipping tt asymmetries at the Tevatron and the LHC", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 86, no. 5, pp. 054022-1-054022-6, 2012.
- 54. Svjetlana Fajfer, Jernej Kamenik, Blaženka Melić, "Discerning new physics in *tī* production using top spin observables at hadron colliders", *J. high energy phys.*, vol. 2012, no. 8, pp. 114-1-114-31, 2012.
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1. Tine Curk, Franziska Matthäus, Yifat Brill-Karniely, Jure Dobnikar, "Coarse graining escherichia coli chemotaxis: from multi-flagella propulsion tologarithmic sensing", In: *Advances in systems biology*, (Advances in experimental medicine and biology, 736), Igor I. Goryanin, ed., Andrew B. Goryachev, ed., New York [etc.], Springer, cop. 2012, pp. 381-395.

- 2. Mojca Čepič, "Flexoelectricity in chiral polar smectics", In: *Flexoelectricity in liquid crystals: theory, experiments and applications,* Ágnes Buka, ed., Nándor Éber, ed., London, Imperial College Press, 2012, pp. 137-176.
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- 4. Marija Mitrović, Bosiljka Tadić, "Emergence and structure of cybercommunities", In: *Handbook of optimization in complex networks: communication and social networks*, My T. Thai, ed., Panos M. Pardalos, ed., New York, Springer, 2012, pp. 209-227.
- 5. Saša Svetina, "On the vesicular origin of the cell cycle", In: *Genesis in the beginning: precursors of life, chemical models and early biological evolution*, (Cellular origin, life in extreme habitats and astrobiology, Vol. 22), Joseph Seckbach, ed., Dordrecht [etc.], Springer, 2012, pp. 757-773.

MENTORING

- 1. Klemen Bohinc, *Including solvent-mediated interactions into the Poisson-Boltzmann theory:* doctoral dissertation, Maribor, 2012 (mentor Sylvio May; co-mentor Milan Brumen).
- 2. Andrej Dobovišek, *Mathematical modelling of the impact of non*steroidal anti-inflammatory drugs on aspirin intolerance in asthma: doctoral dissertation, Ljubljana, 2012 (mentor Milan Brumen; comentor Aleš Fajmut).
- 3. Jure Drobnak, *Constraints on new physics from top quark decays at high precision:* doctoral dissertation, Ljubljana, 2012 (mentor Svjetlana Fajfer; co-mentor Jernej F. Kamenik).
- Ana Hočevar, Lipid vesicle aggregates as models of simple animal tissues: doctoral dissertation, Ljubljana, 2012 (mentor Primož Ziherl).
- Marija Mitrović, Structure and dynamics of techno-social networks: doctoral dissertation, Beograd, 2012 (mentor Bosiljka Tadić).
- Gregor Trefalt, A new synthesis route to Pb(Mg_{1/3}Nb_{2/3})O₃-based materials by the controlled agglomeration of reagent particles: doctoral dissertation, Ljubljana, 2012 (mentor Marija Kosec; co-mentor Bosiljka Tadić).
- 7. Lev Vidmar, *Influence of phonons on physics of strongly correlated electron systems:* doctoral dissertation, Ljubljana, 2012 (mentor Janez Bonča).
- 8. Tine Curk, *Colloidal ordering on soft coated surfaces:* master's thesis, Maribor, 2012 (mentor Jure Dobnikar; co-mentor Francisco Martinez-Veracoechea).

DEPARTMENT OF LOW AND MEDIUM ENERGY PHYSICS

The Department of Low and Medium Energy Physics is active in research relating to atomic physics (low energy physics) and nuclear physics (medium energy physics). The acquired knowledge is applied for monitoring the ionizing radiation in the environment, as well as for interdisciplinary research with ion and photon beams. An important segment of the activities is dedicated to the development of the detection methods for ionizing radiation and the associated instrumentation. The ion accelerator at the department is one of the largest research facilities in the country. The department invested considerable efforts in the development of its own research instrumentation, that enable a specific dual research process: researchers from the department are performing research at major research facilities abroad, and researchers from the European research area are accessing the instrumentation at the JSI ion accelerator in the frame of the Transnational Access Program within 7th FP EU.

F-2



In the field of atomic physics, we have continued the research on the quantum interference of indistinguishable Head: electron pairs emitted upon electron impact excitation or the photoionization of noble-gas atoms. An extensive Asst. Prof. Matej Lipoglavšek theoretical modelling of the exchange interference effects for M_{45} - N_1N_{23} Auger decay in krypton and N_{45} - O_1O_{23} decay in xenon was performed, as well as a comparison with angle-resolved data taken at ELETTRA and angle-integrated (x,2e) coincidence data taken at SOLEIL. We have explained previously the measured fluorescence spectra of helium singly excited states with a theoretical treatment of the atomic system under a combined effect of DC electric field and spin-orbit interaction (*Phys. Rev. A*). We have finished the modelling of the metastable atom yield upon the "box" photoexcitation of helium singly excited states as a function of the magnitude of a DC electric field.

In 2012 we have prepared, for the first time, an experiment on the "finish" beamline I411 operational at the Max-lab in Lund (Sweden) in collaboration with Oulu University. We have measured the yield of photoelectrons, Auger electrons and positive ions as a function of the incoming photon energy scanning over the chlorine L threshold for seven different chlorinated carbohydrates. In March 2012 we visited a commissioning experiment at the new Low Density Matter (LDM) beamline at Elettra new free electron laser. The acquired experience was essential for the preparation of the experimental proposal "Multi-photon excitation of He doubly excited states", which was approved on the first international open access competition for FERMI and will take place in February 2013.

In 2012 we were involved in accurate measurements of the 1s4p and 1s3d multi-electron excitations in the vicinity of the Kr K absorption edge, which were performed at the 6-2 beamline of the SSRL synchrotron, as well as measurements of the Kb^h hypersatellite lines (1s²-1s3p radiative transitions) fine structure were performed for several different V and Cr oxides. At the SuperXAS beamline of the SLS synchrotron in Switzerland, the magnetic circular dichroism (MCD) was measured in order to study the influence of the externally applied magnetic field on the electronic structure of the material. With high-resolution x-ray spectroscopy with proton excitation (HR-PIXE) high-resolution KB (core-valence) emission measurements of chlorine in fine fraction aerosol samples were measured to access the chemical speciation of chlorine in atmospheric aerosols samples, which is key information in source attribution and toxicity study of chlorine-containing particulate matter.

5 eV) m energy Electron 50 Electron energy A (eV)

Figure 1: An excerpt of an angle-integrated electron-electron coincidence energy map of xenon acquired by the Magnetic-Bottle TOF spectrometer in 10 min at 90 eV photon energy (M. Žitnik et al., accepted for publication in Phys. Rev. A).

In 2012 a paper on the design and performance of our curved-crystal spectrometer for high-resolution spectroscopy in the tender x-ray range was published in the field of scientific instrumentation (Rev. Sci. Instrum.). We have also published a review on the results of the resonant inelastic x-ray studies on atoms and simple molecules performed with our spectrometer in recent years (*J. Electron Spectroscopy*). Besides our gas-phase studies, the results of x-ray emission (XES) measurements of S in model glasses used for vitrification of high-level radioactive wastes, performed in collaboration with a group from University of Sheffield, were also



Figure 2: The velocity map image formed by exciting the ground-state atom to the 1s5p ¹P state ($h\omega 1 = 24.046 \text{ eV}$) and ionizing with laser radiation of photon energy $h\omega 2 = 1.772 \text{ eV}$. The main part of the Above the Threshold Ionization (ATI) signal corresponds to the photoelectrons of 1.21 eV energy (outer ring in lower part of the figure). Seen are also photoelectrons at lower kinetic energy of 0.08 eV that originate from 1s3s ¹P state, populated by a spontaneous decay of the 1s5p state. (P. O'Keeffe et al., New J. Phys. 15, 013023, 2013).

published (*Journal of Nuclear Materials*). In collaboration with Uppsala University we have published the results of high-resolution Fe and Zr XES measurements used to study the electronic structure of amorphous $Fe_{100x}Zr_x$ films and multilayers (*J. Phys.: Condens. Matter*). Together with colleagues from the University of Fribourg we have reported on the surface-sensitive grazing emission X-ray fluorescence technique (GEXRF) to determine depth elemental profiles of Al-implanted Si wafers (*X-ray Spectrom.41,98-104*).

Intensive research with ion beams was carried out in 2012 at the ion accelerator Tandetron. Using the ion microbeam, and in collaboration with researchers from the Biotechnical Faculty of the University of Ljubljana, we have carried out a sequence of measurements on slices of biological tissue prepared by the fast freezing and liofilisation technique. In collaboration with "Université catholique de Louvain" (Belgium), we have studied a distribution of iron and other microelements in rice as well as the natrium take-up mechanisms of tomato planted in salted ground. We have continued research on the effects of the redistribution of natrium and chlorine in salted dessert earth and of the gradient of salinity on the root growth (accepted for publication in Nucl. Instr. Meth. B). We demonstrated the efficiency of the micro-PIXE method in following quantitatively the process of heavy-metal uptake by Typha latifolia plant, in collaboration with the Helmholtz centrum from Munich. (accepted for publication in J. Haz. Mat.). We have successfully performed measurements of elemental maps of frozen hydrated tissue slices, as an alternative to freeze dried samples (accepted for publication in Nucl. Instr. Meth. B). In collaboration with the Military Medical Academy, Belgrade (Serbia) we have studied the uptake of golden nanoparticles into human macrofags. We were able to specify the uptake with an accuracy of 1 picogram (accepted for publication in Nucl. Instr. Meth. B).

We have successfully installed a new ion time-of-flight spectrometer that will be used for a new MeV SIMS method – we want to measure the ion yield emitted from the specific target location that is hit by the ion microbeam to obtain information complementary to the that contained in elemental maps measured by the micro-PIXE method. The instrument was built by the IJS Workshop and for the first experiments a pulsed beam of 8 MeV Cl⁷⁺ ions was chosen.

With the significant help of ARRS we have bought and installed in 2012 a new ion source of the "multicusp" type which creates a bright beam of negative hydrogen ions that are subsequently injected into the ion acceleration stage. The beam reaches 15-times larger brightness than the old "duoplasmatron" ion source. With the new proton beam coupled to the microbeamline optics, the 100 pA proton current can be focused down to a beam cross-section of the order of a few hundreds of nanometres.

In the frame of the 7th FW EU SPIRIT we have given access to European researchers to the JSI ion beam infrastructure. We hosted four projects with international access that were performed by researchers from Belgium, Israel, Serbia and the United Kingdom.

In collaboration with the Centre of Excellence CO NOT a series of *in situ* experiments XANES and EXAFS on Li-ion $(\text{Li}_2\text{Mn0}_2\text{Fe}_{0.8}\text{PO}_4)$ in Li_2MnPO_4) and Li-sulphur (Li_2Sx) cathode materials for batteries with a high energy density were performed. The XAS spectra were recorded during the reduction and oxidation of materials with C/15 dynamics and during heating in air up to 400 °C. They register the change of valence of Mn and Fe, and the formation of Li_2S_x compounds during the processes, providing the key information on the battery dynamics and opening the way to optimization of the synthesis of the material with maximum capacity. We continued the long-term project, in collaboration with the Institute of Chemistry and CO-NOT, which involves XAS measurements on the catalytic mesoporous molecular sieves doped with Ca, Cr, Mn, Fe, Ni and Cu, containing also organic building units and on CuPd catalysts. In collaboration with the Laboratory for Material Research of the University of Nova Gorica we published a paper with high impact in Advanced Functional Materials about the doping site of Mn in the crystal structure of strontium titanate, to explain the anomalous magnetic properties of the materials. We continued dynamic activity in the field of fusion research coordinated by EFDA. The work is ongoing within two projects with the Slovenian Fusion Association (SFA – Association EURATOM- MESCS): "Processes with Neutral

Hydrogen Atoms and Molecules" and "Application of Ion Beam Analytical Methods to the Studies of Plasma Wall Interactions in Tokamaks". The work on these projects was directed by three EFDA tasks in close collaboration with IPP, Garching, Germany, CEA, Cadarache, France and INFLPR, Bucharest, Romania. Our particular research interest is in studying the processes occurring during the interaction of neutral hydrogen and deuterium atoms with materials in real time and *in-situ*. We are measuring the hydrogen and deuterium concentrations during the material's exposure to a beam of atomic deuterium. For the purpose of these studies we incorporated an additional diagnostic technique, Nuclear Reaction Analysis at the broad beam ERDA/ RBS experimental station at the JSI ion accelerator. Particularly important are the first *in situ* measurements on damaged tungsten, where the dislocations were induced, similar to those induced by neutron irradiation in ITER. An active collaboration with CEA, Cadarche has been started to understand the thermo-desorption of deuterium from tungsten and the cleaning procedures using surface techniques.

Within our collaboration at the ALOISA beamline group at the Elettra synchrotron (Laboratorio TASC IOM-CNR, Trieste, Italy) we studied the ordering and electronic properties of nanostructured and hybrid organic interfaces. Within our collaboration at the ALOISA beamline of Elettra at the ID26 beamline at ESRF (M. Kavčič et al., Rev. Sci. Instrum., 83, synchrotron (Lab. IOM/CNR), we investigated the electronic structure of 033113, 2012). hetero-organic interfaces and hybrid nanostructures. (PCCP. Phys. chem.



Figure 3: The 2p3d RIXS plane for the tetrahedrally coordinated Na "MoO" system around the Mo LIII edge recorded with our spectrometer

chem. phys. 2012). Our studies of carrier transport over empty molecular orbitals in pi-coupled aromatic molecules evidenced the role of the spatial overlap between adjacent molecular systems in setting the timescale for electron transport across the stack. We found that in ultrathin films of 2,2- and 4,4-paracyclophane molecules, the spatial coupling of pi-conjugated orbitals residing on phenyl rings 3 Å and 4 Å apart, allows electron transfer in 2±0,5 fs and >50 fs, respectively, which is the first direct measurement of through-space charge-transfer dynamics between π -stacked aromatic rings. (*Nature Commun.*).

We studied the properties of different materials by measuring their hyperfine magnetic and electric fields using Mössbauer spectroscopy. Our interest was focused on the properties of magnetic nanoparticles and cathode materials for lithium batteries. This year a project "In-situ NRS mapping of iron based composite electrode materials for Li-ion batteries" at Petra (Hasylab Hamburg) has been approved. The structure and cation distribution in LiFeBO, have been investigated using high-resolution synchrotron X ray diffraction, total scattering data in combination with Mössbauer in ⁶Li NMR spectroscopy.

The laboratory for x-ray fluorescence spectrometry has mostly dealt with measurements concerning quantification of elemental composition in plants on the cellular level in collaboration with Cathedra for plant physiology at the Biotechnical Faculty, University of Ljubljana, using mainly the x-ray synchrotron light to acquire the XRF spectra. At the TwinMic beamline of ELETTRA, we studied the localisation of silicon, arsenic and selenium in plant tissues by analysing the intensity of the Si-K, As-L, and Se-L, spectral lines. At the ESRF synchrotron in Grenoble (France), we collaborated with the Biotechnical Faculty, University of Ljubljana, to examine how cadmium affects the metabolic paths in plant roots.

In the field of archaometry we were mainly studying semi-precious stones embedded in archaeological objects. In collaboration with the Museum of Natural History we analysed all the emeralds excavated in the territory of Slovenia and found that they very likely originate from Egypt and possibly Afghanistan. A large number of analyses were made on garnets, which were a popular form of jewellery used during the People Migration period. All the analysed garnets were classified as almandine, whose origin may be in India and Ceylon. It is interesting that we did not encounter Bohemian pyropes that only appear at Merovingian sites of the 7th Century. In the field of glass analysis we studied glass from the period of the late 19th-early 20th Century, which was significantly pigmented by uranium salts and colloidal gold or copper. Following the analytical results and written sources, we were able 27, 834, 2012).



Figure 4: Surface-topography reconstruction of Ca in seashell by stereo-PIXE. Individual distribution of Ca K α line yield taken from the X-ray detector positioned (a) left and (b) right with respect to the beam direction. Surface inclination reconstruction by means of stereo X-ray images (c). Lateral inclination profile across the horizontal direction in the centre of the map (d) (E. Gholami Hatam et al., J. Anal. At. Spectrom.,



Figure 5: Resonant photoemission (RPES) intensity map of LUMO and LUMO + 1 resonances of multilayer (a) and monolayer (b) of [2,2] paracyclophane (22PCP). (c) Line profiles of LUMO resonances for monolayer (red) and multilayer (blue) 22PCP with the valence band spectrum (dashed blue, 140 eV photon energy). (A. Batra et al., Nature Commun. 3, 1086, 2012).

to recognize the glass imported from Bohemia and glass produced in local glassworks of Pohorje and Hrastnik.

In the field of nuclear physics, we have continued the measurements within the A1 Collaboration at MAMI (Mainz, Germany) with the new KAOS spectrometer, which allows for the detection of positively and negatively charged reaction products up to momenta of 1.5 GeV/c. We have also continued to perform several calibrations of electroproduction of charged kaons and the formation of hyperons in nuclei, as well as kaon electroproduction on proton targets. We have started to design and construct the second aerogel Cherenkov counter that is to be positioned into KAOS behind the existing scintillator walls and that is envisioned to increase the efficiency of kaon/ pion separation at high counting rates occurring at a zero scattering angle. We have continued the data analysis of the high-precision double-polarization measurement of electroproduction of neutral pions on protons in the region of the Roper resonance. We have also extended the experiment on virtual Compton scattering to several points along the momentum transfer axis, with the aim of ultimately determining the electric and magnetic generalized polarizabilities or their specific linear combinations.

In the framework of the Hall A Collaboration at Jefferson Laboratory we have performed two sets of measurements. We have collaborated in the run group of E08-007 and E08-027 experiments in which we have investigated the elastic form-factors of the proton and the polarized structure function g2p. We have finished the optical calibration of the BigBite spectrometer, which was also used in the E05-102 experiment.

We investigated the effect of the electron screening in nuclear reactions. Electron screening enhances the nuclear reaction cross-sections at low energies compared to the cross-sections for reactions between bare nuclei, stripped of all their atomic electrons. In reactions in the laboratory, the nuclei are always accompanied by electrons and therefore, electron screening cannot be avoided. On the other hand, in stellar plasma, where for example nucleosynthesis occurs, the conditions are very different and we would like to know the cross-sections for reactions between bare nuclei that cannot be directly measured on Earth. To improve the understanding of electron screening, we compared the proton capture probabilities in metallic nickel and insulating nickel oxide targets. The probabilities were determined from

the yields of characteristic γ rays produced in different nuclear reactions. The γ rays were measured with in-beam high-resolution γ -ray spectroscopy at the JSI ion accelerator. Our results showed that the probability for the (p,n) reaction is larger in a metallic than in an insulating target. We also showed that the probability for the (p, γ) reaction is larger in metallic than in an insulating target.

With colleagues from the Communication Systems Department and from the institute GSI in Darmstadt, fundamental work on methods for fast algebraic computation and the acquisition of nuclear spectroscopic pulses was further extended. One of the most efficient of the above techniques was adapted for the first time to the highenergy resolution scintillators LaBr:Ce. We have developed a new method for adaptive triggering in scintillation detectors that significantly extends the dynamic range of particle energy measurements with scintillators. The above techniques were transferred into the biomedical field, within the Regional Competency Centre for biomedical engineering. In collaboration with the company Instrumentation Technologies we further developed their recent product for digital pulse processing. In another collaboration with Beyond Semiconductor Ltd we started to shape a novel compensation method for saturation artefacts in multi-pixel photon counters.

In collaboration with the Department of Theoretical Physics at the JSI and University of Coimbra, we investigated dynamical (electromagnetic and weak) processes on protons and neutrons in the energy region of the Roper resonance and of the negative-parity resonances.

In 2012 we continued with the detection of tritium in waters, which serves as an effective indicator of water dating. More than 40 percent of all the water resources in Slovenia are not yet characterized for their tritium content, therefore we continued with systematic sampling and measurements. As the tritium content in the atmosphere is decreasing globally, this is also the case for precipitation and consequentially for the subterranean waters, we improved the phases in the tritium detection method with electrolysis enrichment. The samples with such low concentrations require specific treatment, therefore we started with the Bayesian statistics approaches for the determination of the radionuclide concentrations.

As the European Union is subsidizing the application of biofuel with tax reductions for the producers and the distributors, several methods were developed to monitor the fuel composition. In 2012 we started to develop a direct LSC method for the biocomponents in fuel.

In addition to the basic science activities, the department was active in conducting the radiological monitoring of the living environment in Slovenia, radiological monitoring of fodder in Slovenia, regular off-site radiological monitoring around Krško NPP, central radioactive waste repository radiological monitoring, monitoring of the radioactivity in drinking water, calibrations of the radiation gauges and TLD measurements of the personal and environmental doses. The laboratories active in the radiological monitoring are certified according to the ISO 17025 standard.

Last year, we have successfully launched a new project entitled "Testing Services for Filter Media used and the IMS Radionuclide Stations" funding by an international organisation CTBTO.

In 2012 we were awarded a 3-year European project under FP7-



Figure 6: Lateral elemental distributions in the cross-section of the tartary buckwheat (Fagopyrum tartaricum) measured with micro-PIXE technique at the JSI ion accelerator. The images are obtain by scanning of 2.5 MeV proton beam with diameter of 1.2 micrometres. Scan size 2.2 x 2.2 mm². Work done in collaboration with Paula Pongrac and coworkers from Biotechnical Faculty of University of Ljubljana.

Fission-2011 entitled "Innovative integrative tools and platforms to be prepared for radiological emergencies and post-accident response and Europe" with the specific task "Table-top exercise on monitoring a large-scale cross-border contamination".

In 2012 we intensified the cooperation with Metrology Institute of the Republic of Slovenia. Our work received very good reviews, which consequently increased financial income. As a designated institution and as the holder of the national standard for the field of ionizing radiation in Slovenia, we are taking part in a new EU funding EMRP project "Metro materials with elevated natural radioactivity".

Members of the Infrastructure Group also took part in regular drills and special tasks with the radiological mobile unit.

Some outstanding publications in the past year

- Gajić-Kvaščev, Maja, Marić Stojanović, Milica, Šmit, Žiga, Kantarelou, Vasoliki, Germanos Karydas, Andreas, Šljivar, Dušan, Milovanović, Dragan, Andrić, Velibor. New evidence for the use of cinnabar as a colouring pigment in the Vinča culture. J. archaeol. sci., 2012, vol. 39, 1025-1033.
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- 11. Novak, Sara, Drobne, Damjana, Valant, Janez, Pipan Tkalec, Živa, Pelicon, Primož, Vavpetič, Primož, Grlj, Nataša, Falnoga, Ingrid, Mazej, Darja, Remškar, Maja. Cell membrane integrity and internalization of

ingested TiO₂ nanoparticles by digestive gland cells of a terrestrial isopod. Environ. toxicol. chem., 2012, vol. 31, 1083-1090.

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Patent granted

1. Roman Novak, Matjaž Vencelj, Method for quantum distribution of the short-range key, SI23596 (A), Urad RS za intelektualno lastnino, 29.6.2012.

INTERNATIONAL PROJECTS

- 1. Calibrations
- Matjaž Mihelič, M. Sc.
- Provision of testing services for filter media used in IMS radionuclide stations The Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization Dr. Benjamin Zorko
- 7. OP MC-PAD: Marie Curie training network on particle detectors; PITN-GA-2008-214560 European Commission
- Jure Beričič, B. Sc.
- 7. FP SPIRIT: Support of public and industrial research using ion beam technology European Commission Asst. Prof. Primož Pelicon
- 7. OP EURATOM: Application of ion beam analytical methods to the studies of plasma wall interaction in Tokamas 1.4.3.-FU; Annex 2 to Contract 3211-08-02; FU07-CT-2007-00065
 Ministry of Higher Education, Science and Technology
- Asst. Prof. Primož Pelicon
- FP EURATOM: Process with neutral hydrogen atoms and molecules, 1.4.1.-FU; Annex 3 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology
- Dr. Iztok Čadež
 7. FP EURATOM: H2-D2 Molecule wall interaction, 1.4.1.-FU; Annex 4 to Contract 3211-08-000102, FU07-CT-2007-00065
- Ministry of Higher Education, Science and Technology Dr. Iztok Čadež
- FP EURATOM, MHEST Association: D re-adsorption/re-saturation of W surfaces subjected to helium RF-discharge as a fuel removal technique; WP12-IPH-A03-2-06/PS-01 Ministry of Education, Science, Culture and Sport Asst. Prof. Primož Pelicon
- 7. FP EURATOM, MHEST Association: Atomic and low-energy hydrogenic plasma interaction with damaged tungsten; WP12-IPH-A03-1-13/PS-01 Ministry of Education, Science, Culture and Sport Asst. Prof. Primož Pelicon
- 10. MetroRWM: Metrology for radioactive waste management Euramet e. V.
- Branko Vodenik, M. Sc.
- 11. MetroMetal Ionising radiation metrology for the metallurgical industry Euramet e. V.
- Branko Vodenik, M. Sc.
- Convention de mise a disposition; Letter N/REF: NS/MD/CONV/04FRE2681JS/2004 dtd. 8. 9. 2004
 - École Normale Superieure
 - Dr. Iztok Čadež
- 13. COST CM0805: The Chemical Cosmos: understanding chemistry in astronomical environments
 - COST Office Dr. Iztok Čadež
- Studies of short-range correlations Slovenian Research Agency
- Prof. Simon Širca
- Dynamics at nanoscale Slovenian Research Agency Asst. Prof. Matiaž Žitnik
- ISC methods for determination of H-3 and C-14 in environmental samples Slovenian Research Agency
- Dr. Jasmina Kožar Logar 17. Measurements and control of deuterium in fusion material Slovenian Research Agency
- Asst. Prof. Primož Pelicon 18 Co-financing of the promotion of scien
- 18. Co-financing of the promotion of science

Slovenian Research Agency Asst. Prof. Primož Pelicon

RESEARCH PROGRAMS

- 1. Archaeological and archaeometric research of portable archaeological heritage Prof. Žiga Šmit
- 2. Object and prestige; taste, status, power (researches of the material culture in Slovenia) Dr. Marijan Nečemer
- 3. Structure of hadronic systems
- Prof. Simon Širca Studies of atoms molecu
- Studies of atoms, molecules and structures by photons and particles Asst. Prof. Matjaž Žitnik

R & D GRANTS AND CONTRACTS

- Investigation of plant ion homeostasis using elemental imaging by laser ablationinductively coupled plasma mass spectrometry (basic research project) Asst. Prof. Primož Pelicon
- 2. Research of the ionome of selected mycorrhizal plants Asst. Prof. Primož Pelicon
- Sustainable land use in relation to soil and crop quality Asst. Prof. Primož Pelicon
- 4. Archaeologies of hunter-gatherers, farmers and metallurgists: cultures, populations, palaeoeconomies and climate
- Dr. Marijan Nečemer 5. Development of Cherenkov radiation detector
- Prof. Simon Širca
- 6. Groundwater age determination in deep aquifers of Slovenia Dr. Jasmina Kožar Logar
- Complex hyperspectral system for automatic analysis and ccontrol of pharmaceutical pellet coating processes Dr. Peter Kump
- Center of competence biomedical engineering: CC BME Dr. Matjaž Vencelj

NEW CONTRACTS

- 1. Off-site radiological monitoring of NPP Krško 2011-2013 Krško Nuclear Power Plant
- Asst. Prof. Matej Lipoglavšek 2. TLD Dosimetry service
- General Hospital , 'Dr. Franc Derganc'' Boštjan Črnič
- Ecology laboratory with mobile unit Ministry of Defence
 - Asst. Prof. Matej Lipoglavšek
- Annex No. 7 to the contract on performing activities and fulfillment of obligations of holder of national standard in the field of ionising radiation Ministry of Economic Development and Technology Matjaž Mihelič, M. Sc.
- Maintenance of radiological emergency preparedness for a period of 5 years (2012-2017)

Krško Nuclear Power Plant

Asst. Prof. Matej Lipoglavšek

VISITORS FROM ABROAD

- Mr. Sergej Tomić, Institute for Medical Research, Military Medical Academy, Belgrade, 1. Serbia, 13.-17. 7. 2012
- 2 Dr. Luis Miguel Rodriguez, Centro Atómico Bariloche, Bariloche, Argentina, 3. 5.-31. 7. 2012
- Mr. Daniél Slenders, Katholieke Universiteit Leuven, Zonhoven, Belgium, 7. 4.–26. 8. 2012 Mr. Ian Stokes, Keele University, Keele, Great Britain, 16.–22. 7. 2012 3.
- 4.
- Dr. Olga Ogorodnikova, IPP, Garching, Germany, 13.-22. 8. 2012 5

STAFF

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- Prof. Iztok Arčon*
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- 5 Denis Glavič Cindro, M. Sc.
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- Asst. Prof. Matjaž Kavčič
- 8 Prof. Alojzij Franc Kodre*, retired 01.10.12
- 9 Dr. Peter Kump
- 10. Prof. Andrej Likar*

11. Asst. Prof. Matej Lipoglavšek, Head

- 12. Dr. Andrej Mihelič
- 13. Dr. Marijan Nečemer
- 14. Asst. Prof. Primož Pelicon
- 15. Zdravko Rupnik, M. Sc.
- 16. Prof. Simon Širca*
- 17. Prof. Žiga Šmit*
- 18. Dr. Matjaž Vencelj
- 19. Branko Vodenik, M. Sc.
- 20. Asst. Prof. Matjaž Žitnik
- Postdoctorial associates
- 21. Dr. Jasmina Kožar Logar
- 22. Dr. Sabina Markelj
- 23. Dr. Paula Pongrac, left 01.02.12
- 24. Dr. Benjamin Zorko

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- 2. A1 Collaboration: Patrick Achenbach et al. (36 authors), "Strange hadronic physics in electroproduction experiments at the Mainz Microtron", Nucl. phys., Sect. A, vol. 881, pp. 187-198, 2012.
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- Mr. Oren Shelef, Ben-Gurion University of the Negev, Sede Boqer Campus, Izrael, 7. 11.-22. 9. 2012
- Dr. Isabelle Lefevre, Univerite catholique de Louvain, Louvain-la-Neuve, Belgium, 8 11.-16. 12. 2012

Postgraduates

- 25. Jure Beričič, B. Sc.
- 26. Rok Bohinc, B. Sc.
- 27. Helena Faifar**
- 28. Jelena Gajević, B. Sc.
- 29. Dr. Nataša Grlj, left 01.07.12
- 30. Luka Jeromel, B. Sc.
- 31. Katarina Kovačič, B. Sc. 32. Dr. Miha Mihovilovič, left 01.04.12
- 33. Mojca Miklavec, B. Sc.
- 34. Samo Štajner, B. Sc.
- 35. Anže Založnik, B. Sc.
- **Technical officers**
- 36. Boštjan Črnič, B. Sc.
- 37. Matjaž Mihelič, M. Sc.
- 38. Primož Vavpetič, B. Sc
- Technical and administrative staff 39. Drago Brodnik
- 40. Mojca Gantar
- 41. Sandi Gobec
- 42. Zvonimir Grabnar
- 43. Mirko Ribič, B. Sc.

Note:

- * part-time JSI member postgraduate financed by industry
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PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

 Andrej Mihelič, Matjaž Žitnik, P. O'Keeffe, Paola Bolognesi, Angelica Moise, R. Richter, Lorenzo Avaldi, "Studies of multiphoton processes in noble gas atoms", In: *Contributed papers & abstracts of invited lectures, topical invited lectures and progress reports,* 26nd Summer School and International Symposium on the Physics of Ionized Gases, SPIG 2012, August 27th - 31st, 2012, Zrenjanin, Serbia, Milorad Kuraica, ed., Zoran Mijatović, ed., Novi Sad, University of Novi Sad, Faculty of Sciences, Department of Physics, cop. 2012, pp. 012016-1-012016-8.

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INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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PATENT

1. Roman Novak, Matjaž Vencelj, *Method for quantum distribution of the short-range key*, SI23596 (A), Urad RS za intelektualno lastnino, 29.6.2012.

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- Luka Debenjak, Construction and calibration of the Čerenkov radiation detector for high-countrate hypernuclear experiments: doctoral dissertation, Ljubljana, 2012 (mentor Simon Širca).
- 2. Nataša Grlj, Development of the confocal PIXE set-up for multielemental depth resolved measurements and three-dimensional microscopy: doctoral dissertation, Nova Gorica, 2012 (mentors Primož Pelicon, Matjaž Žitnik).
- Gregor Kladnik, *Electronic structure and charge transfer at nanostructures and hybrid interfaces:* doctoral dissertation, Ljubljana, 2012 (mentor Dean Cvetko).
- 4. Miha Mihovilovič, Measurement of double polarized asymmetries in quasi-elastic processes ³He(e, e'd) and ³He(e, e'p): doctoral dissertation, Ljubljana, 2012 (mentor Simon Širca; co-mentor Douglas W. Higinbotham).
- Mitja Blažič, System test of radio frequency and clock generator: master's thesis, Nova Gorica, 2012 (mentor Iztok Arčon).

DEPARTMENT OF THIN FILMS AND SURFACES

F-3

The main research field of the department is the development, deposition and characterization of hard protective PVD coatings, while research is also conducted in other fields of thin films and surface physics. The basic research is concentrated on the study of the physical and chemical properties of various multicomponent, multilayer and nanostructured coatings. Among the applied research, different coatings are developed for the protection of tools for various production processes in industry.

Throughout the year, the research and development work of the department has remained concentrated on the field of hard protective coatings. The majority of the work was of an applied nature and in many cases connected to the industrial implementation of hard coatings, failure diagnostics and interpretation, and the solving of specific industrial problems.

Today's trend of hard-coating development is in the area of nanostructured systems, i.e. nanolayer and nanocomposite coatings. One of these systems is the (Ti,Al,Si)N, which has been studied for the past few years, and Head: which we last year successfully implemented in industrial production. The formation of a nanocomposite coating is Dr. Peter Panjan only possible if the kinetical conditions of spontaneous phase separation are met. In our case these are TiN or TiAIN grains of about 10 nm size in a matrix of amorphous Si₁N₄. The coating was extensively analyzed by transmission electron microscopy, and the results compared to the numerical modeling of thin-film growth. This contribution was given by Aleksandar Miletić (University of Novi Sad, Serbia), as it is the topic of his PhD thesis.

The system (Ti,Al,Si)N is nowadays used in several tens of companies in Slovenia; it proved to be specifically

suitable for the protection of cutting tools for hard machining (above 60 HRC). The technological importance of this research is also evident from the fact that in Slovenia, as well as around the world, the share of classic hard coatings (TiN, CrN) is in constant decline. They are being replaced by ternary coatings (TiAlN), and in the past few years by nanolayer and nanostructured coatings.

One of the major problems in hard coating applications is the appearance of defects, which appear during the coating growth and have a negative effect on the corrosion resistance and the tribological properties (increased wear, material sticking). Last year we developed a new technique for studying the defects, which are first exposed to an intensive ion etching. For that purpose we use the technique glow-discharge optical emission spectroscopy (GDOES), which is primarily intended for the analysis of chemical composition. Using this technique we first make a crater where there is an enhanced contrast of defects, which can then be studied by scanning electron microscopy.

This work has been done in collaboration with the Faculty of Mechanical Engineering of the University in Maribor, and is the topic of the PhD thesis of our young researcher Peter Gselman. Using a FIB (focused ion beam), integrated in a conventional scanning electron microscope, we made a series of cuts through the defect. Images of individual cuts were made, to be followed by a 3D reconstruction of several defects (craters, spherical droplets, pores). We found that by volume the average analysed defect size is only one-third that of the damaged substrate size, which was exposed to the corrosion medium.

For studying the influence of stoichiometry on ternary coating properties we made several tests using so-called triangular targets. The idea is to substitute a monolithic target with a pair of triangular targets of different composition, which enables the deposition of a composition gradient along the chamber's vertical axis. In this way a set of samples with different composition is deposited in a single process. The first, more extensive analysis was done in the concentration gradient $Cr_v V_{1,v} N$. We found an important dependence of texture and grain size on the chromium-to-vanadium ratio (i.e., on the sample height

In 2012 we acquired a patent for a nanolayer

23538: Hard protective coatings with the ability

blue coating based on AITiN/TiN (patent no.

to change their colour).

Figure 1: Cross-section TEM micrograph of the blue nanolayer coating AlTiN/TiN (image author: Asst. Prof. Goran Dražić)

within the chamber). However, the mechanical properties (hardness, adhesion) only marginally changed with composition. Going the classic way (using monolithic targets), 20 individual depositions would be needed, while by applying the triangular targets only one deposition was necessary. The application of this method is a topic of

absorp reflection layer TiN protective layer 50 nm AITIN/TIN 30 nm



Figure 2: Low-angle cross-section across a defect in the CrN/TiAlN multilayer coating, which evolved from several seeds



Figure 3: SEM micrograph of a defect in the multilayer coating CrN/ TiAlN, formed at the edge of a GDOES crater (glow discharge optical emission spectroscopy)



Figure 4: Micrograph of a defect in the TiAlN coating, acquired by the focused ion beam (image author: Dr. Tonica Bončina)

our young researcher Aljaž Drnovšek, who will concentrate on the system $\operatorname{Cr}_{x}\operatorname{Al}_{1-x}$ N, with later additions of another metallic element (e.g., vanadium, titanium, silicon).

Coatings with a low friction coefficient are also interesting. Last year Dr. Srečko Paskvale defended his PhD thesis "Carbon-based protective coatings deposited by physical vapour deposition processes", where he analysed the tribological properties of coatings with a low friction coefficient, prepared by different deposition techniques. Most emphasis was given to the bilayer coating TiAlN/a-CN_x, which was successfully implemented in industrial production. In his work he analysed the dependence of the friction coefficient and the wear parameters on the deposition parameters (thickness, rotation rate and sample position in the chamber), and surface condition (roughness, defect density).

Nanolayer and nanocomposite coatings are also a topic of the Nano Tool project (ERA-SME). Within this project we are developing coatings for the protection of cutting and forming tools under specific wear conditions. We analysed in detail the influence of the cutting edge's condition on the coating quality. Partners from the Vienna University of Technology tested the behaviour of the coated cutting tools in real conditions.

The department is involved in several applied projects, which are cofinanced by individual companies. For the company Impol, d. d., we are developing coatings for two types of applications: for extrusion tools and for final products made of wrought aluminium. For the latter there are promising results using low-temperature TiN prepared by pulsed deposition. Together with the company Magneti, d. o. o., we are developing a coating to protect Sm-Co permanent magnets at elevated temperatures. A promising way goes in the direction of a two-layer structure: the lower one for surface smoothing, and the upper one classic TiN. There are many more informal cooperations with different companies, even after a project has expired. The work is usually done as an investigation, where we solve specific advanced technological problems. For the company Kolektor, d. d., we made a preliminary analysis of the tribological properties of the saw blades, which are used for cutting commutator bodies. In this way we intend to optimize the selection of coatings to minimize wear. We also intensively collaborate with the company Cetis, d. d., where our "young researcher from industry" Vladan Mladenovič is employed. The topic of his work is surface structuring using different machining techniques (scratching, laser treatment, electroerosion) and analysis of these processes at the micro-level.

Tribocorrosion enables simultaneous measurements of the sliding wear parameters (e.g., friction coefficient) and the electrochemical parameters (corrosion potential, corrosion current). In this way we can in-situ follow the degradation of the coating or passive layer on a passive metal. In practical examples of corrosion tests (two coatings TiAgN and TiSiN, and substrate 316L) we showed that tribocorrosion tests can be used for the planning and estimation of coating properties with optimal purposes. In the field of bio-applications we are continuing our studies of corrosion and the tribological properties of diamond-like carbon coatings deposited on stainless-steel substrates.

At the level of basic science we are collaborating with several other industrial partners. Last year Dr. Matjaž Panjan was at a post-doc at Montreal Polytechnic. His research was connected with the development of several nanocomposite hard coatings, prepared by high-impulse power magnetron sputtering. In the scope of this work he is active in two Canadian projects. The first project is "Optimal cutter geometry for the drilling and the trimming

of multilayer material" on the protection of tools for the machining of carbon-fibre-reinforced composites, in collaboration with the companies Bombardier and Minicut, and the university École de Technologie Supérieure. The second project is "Water Erosion Resistant Surface Treatment" on the protection of turbine blades in gas turbines, in collaboration with the companies Rolls-Royce Canada and Patt Technologies, and universities Concordia University and École de Technologie Supérieure.

Dr. Matjaž Panjan had another post-doctoral stay, under the Fulbright fellowship at the Lawrence Berkeley National Laboratory in the USA. He investigated plasma processes which develop during the 100-microsecond-long pulses during high-power impulse magnetron sputtering. Using a high-speed camera (exposition time below 10 ns), mass spectroscopy and ion collectors he studied plasma structures that form close to the cathode and travel in the direction $\mathbf{E} \times \mathbf{B}$. The study of plasma structures and the so-called ionization zones are crucial for understanding the principles of magnetron discharge. These zones are responsible for the transport and spatial distribution of pulsed and classic magnetron sputtering.

We have a bilateral project with the Institute of Physics of the Czech Academy of Sciences, where the primary topic is the deposition and characterization of colour coatings. We performed the optical characterization of our coatings and based on these measurements and the ones performed in



Figure 5: SEM micrograph of V_2O_5 crystals that formed during the oxidation of the (Cr,V)N coating at 750 °C

Canada we were able to explain the physical background of the colour changes in the AlTiN/TiN coatings – the "blue coating", introduced in industry a few years ago. The colour is a consequence of the interference with the first-order reflected ray, spectrally-sensitive absorption in the toplayer and spectrally-sensitive reflection in the reflection layer.

We informally collaborate with several other partners. Together with the Vinča Nuclear Institute from Belgrade we have analysed radiation damage of craters after treatment by laser pulses. We have also continued the work with the Research Institute for Technical Physics and Materials from Budapest; for them we are depositing specific structures for sputtering analytics. In the program Euratom our task is the synthesis of different hydrogenised carbon deposits, which should be as similar as possible to the deposited impurities in a fusion reactor.

Some outstanding publications in the past year

- Čekada, M., Kahn, M., Pelicon, P., Siketić, Z., Bogdanović-Radović, I., Waldhauser, W., Paskvale, S.: Analysis of nitrogen-doped ion-beam-deposited hydrogenated diamond-like carbon films using ERDA/RBS, TOF-ERDA and Raman spectroscopy. Surf. Coat. Technol. 211 (2012), pp. 72–75
- Panjan, P., Čekada, M., Panjan, M., Kek-Merl, D., Zupanič, F., Čurković, L., Paskvale, S.: Surface density of growth defects in different PVD hard coatings prepared by sputtering. Vacuum 86 (2012) 6, pp. 794–798
- 3. Panjan, M., Čekada, M., Panjan, P., Zupanič, F., Kölker, W.: Dependence of microstructure and hardness of TiAlN/VN hard coatings on the type of substrate rotation. Vacuum 86 (2012) 6, pp. 699–702

Patents granted

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- Matjaž Panjan, Miha Čekada, Peter Panjan, Damjan Matelič, Andrej Mohar, Tomaž Sirnik, Jožko Fišer, Hard protective coatings with the ability to change their color, SI23538 (A), Urad RS za intelektualno lastnino, 31.5.2012.

INTERNATIONAL PROJECTS

- 7. FP EURATOM; Plasma Deposition of H:C-metal Coatings 1.4.5.-FU; Annex 3 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Dr. Peter Panian
- Deposition and Characterization of Nanostructured hard Coatings with Tailored Optical Properties Slovenian Research Agency

Asst. Prof. Miha Čekada

RESEARCH PROGRAM

1. Thin film structures and plasma surface engineering Dr. Peter Panjan

R & D GRANTS AND CONTRACTS

- 1. Molecular Motors Dr. Darinka Kek Merl
- Hybrid Nanomaterials for Low-friction Polymer Composites and Energy Conversion Dr. Peter Panjan
- 3. Organic-inorganic thin film structures for electronics components
- Dr. Peter Panjan 4 Materials and structures for ontically variable security devices
- Materials and structures for optically variable security devices Dr. Peter Panjan
- Research and development of rapid production and repair in modern 3D cutting tools with advanced laser technologies Dr. Peter Panian
- Development of new generation of hard coatings with pulsed sputter deposition Dr. Peter Panjan
- 7. Protected Permanent Magnets for Advanced High-Temperature Applications Asst. Prof. Miha Čekada
- Multifunctional Nanostructured Films for Artificial Implants Corrosion and Tribocorrosion Processes Dr. Darinka Kek Merl
- 9. Colour, absorption and protective nanolayer coatings for aluminium alloy Dr. Peter Panjan

- Functionalization of biomedical samples by thermodynamic non-equilibrium gaseous plasma Dr. Peter Panjan
- Toward ecologically benign alternative for cleaning of delicate biomedical instruments Dr. Peter Panjan
- ERASME, NANO-TOOL; Aplication of NANO Coatings on the Vital Cutting Edges and Forming Parts of Progressive and Transfer Tools and Milling Tools for Automotive Production, to increase Productivity, Persistence and Longer Life Time Dr. Peter Panjan

VISITORS FROM ABROAD

- 1. Dr. Rainer Cremer, KCS Europe, Monschau, Germany, 3. 4. 2012
- 2. Aleksandar Miletić, Pal Terek, University of Novi Sad, Novi Sad, Serbia, 14.-18. 5. 2012
- 3. Dr. Rainer Cremer, KCS Europe, Monschau, Germany, 15.-16. 5. 2012
- 4. Aleksandar Miletić, Pal Terek, University of Novi Sad, Novi Sad, Serbia, 30. 7.–3. 8. 2012
- 5. Dr. Michal Novotný, Institute of Physics of the Academy of Sciences of the Czech Republic, Prague, Czech Republic, 6.–10. 11. 2012

NEW CONTRACT

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- Dr. Jiří Bulíř, Dr. Ján Lančok, Institute of Physics of the Academy of Sciences of the Czech Republic, Prague, Czech Republic, 20.–23. 11. 2012
- Dr. Biljana Gaković, Dr. Suzana Petrović, "Vinča" Institute for Nuclear Sciences, Belgrade, Serbia, 3.–7. 12. 2012
- Kateřina Horáková, Institute of Physics of the Academy of Sciences of the Czech Republic, Prague, Czech Republic, 17.–20. 12. 2012

STAFF

Researchers

- 1. Asst. Prof. Miha Čekada
- 2. Dr. Darinka Kek Merl
- 3. Dr. Peter Panjan, Head
- Postdoctorial associates
- Dr. Matjaž Panjan
 Dr. Srečko Paskvale
- Postgraduates
- 6. Aljaž Drnovšek, B. Sc.

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- Technical and administrative staff
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 Andrej Mohar
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DEPARTMENT OF SURFACE ENGINEERING AND OPTOELECTRONICS F-4

The research program is associated with vacuum science, technology and applications. The main activities are focused on plasma science, the modification of advanced biomedical materials and products for improved biocompatibility, the characterization of inorganic, polymer and composite materials with different thin films on the surface, the modification and characterization of fusionrelevant materials, the thermodynamics of trapped gases and methods for sustaining ultra-highvacuum environment, vacuum optoelectronics, and basic research in the field of surface and thin-film characterization by electron spectroscopy techniques.

A variety of low-pressure gaseous discharges have been used to create non-equilibrium plasma suitable for the treatment of solid materials. The research team has specialized in high-frequency discharges. Both radiofrequency and microwave generators are used to create gaseous plasma with suitable characteristics. Radio-frequency discharges are usually coupled inductively in order to take advantage of an electrode-less configuration. The absence of strong electrical fields in such discharges prevents the sputtering of solid materials by energetic ions and thus Head: the preservation of the original surface properties of the discharge chambers. Such discharges are often used Prof. Miran Mozetič when homogeneous plasma in a rather large volume needs to be created and the low kinetic temperature of the neutral gas needs to be preserved. Microwave discharges, on the other hand, are used where dense plasma should be concentrated into a rather small volume. Plasma driven by microwave generators is created either in a resonant cavity with standing microwaves or in narrow tubes taking advantage of the surface waves propagating along the



tube. The first configuration is characterized by extremely high resonant voltages localized close to the centre of the resonant cavity, while in the other configuration the peak voltage is moderate. Both configurations of microwave discharges never create very cold plasma so they are suitable for the treatment of materials at elevated temperatures. Plasma created by surface waves in narrow long tubes is cooled upon adiabatic expansion due to a pressure gradient along the continuously pumped narrow glass tubes so it is suitable as a convenient source of cold radicals.

Gaseous plasma contains a variety of particles that are used for the treatment of solid materials. Plasma is usually created in gases such as oxygen, hydrogen, nitrogen and ammonia. Gaseous molecules dissociate and partially ionize in plasma so the concentration of neutral as well as ionized reactive particles is orders of magnitude larger than in the equilibrium state of the gas at the chosen temperature. Plasma particles are chemically very reactive and often interact with surfaces of solid materials, even at room temperature. Since the kinetic energy of particles is low the interaction is essentially chemical. The interaction between the plasma particles and solid materials causes a modification of the surface properties, including surface



Figure 1: Plasma is created using an inductively coupled RF discharge

functionalization, low-temperature etching and the spontaneous growth of nanostructures on originally flat surfaces. Although oxygen plasma is nowadays widely used for the surface modification of polymers and other hydrogen-

ated carbon materials the exact mechanisms involved during the interaction of various oxygen reactive particles with organic materials is still far from being well understood. To enlighten this hot topic of current science we organized a specialized workshop entitled "69th IUVSTA workshop on modification of organic materials by excited radicals created in non-equilibrium oxygen plasma". The Workshop was supported by International Union for Vacuum Science, Technique and Applications (IUVSTA) and took place in the small village of Cerklje na Gorenjskem close to Ljubljana International Airport. Invited participants presented different views on this complex phenomenon

A novel method for determining the O-atom density in weakly ionized oxygen plasmas and the afterglows from catalytic probe signals has been developed and applied for the optimization of our sensors, thus expanding their applicability to gases such as carbon dioxide.

and agreed that a lot of work will have to be performed in the future in order to understand the roles that each type of reactive particles play upon the treatment of organic materials with oxygen plasma. The participants agreed that

synergistic effects should not be neglected and stressed the need to have independently adjustable fluxes of specific radicals onto the surfaces of organic materials.

The functionalization of polymer materials with polar functional groups is usually performed by a treatment with non-equilibrium oxygen plasma. Surfaces of many widely used polymers are saturated with functional groups by



Figure 2: Density of O-atoms in the early afterglow of plasma created in CO_{x} Dashed area represents possible values taking into account extreme values of the recombination coefficients and the middle curve the most probable value.

using either positively charged molecular and atomic oxygen ions or neutral reactive species such as atoms in the ground and metastable states. Since the flux of atoms in the ground state is of the highest importance for the proper functionalization of polymer materials we developed a novel method for the determination of the O-atom density in weakly ionized oxygen plasmas and afterglows from catalytic probe signals using the right model based on physical formalism. The probes are also capable of measuring the O-atom density in plasma created in other gases such as carbon dioxide. The treatment of polymers by such radicals allows for a uniform distribution of functional groups on the entire surface of the selected polymer materials. In many practical applications, however, only selected areas should be functionalized. Since methods for localized functionalization at the micrometre scale are not yet known we invented an opposite technique: The polymer sample is first functionalized by plasma treatment and then selected areas are exposed to energetic electrons from an appropriate electron gun. Electrons heat the

surface spot and de-functionalize it since the functional groups are not stable at elevated temperatures. The electron jet raster on the surface and thus a selected area becomes free from polar functional groups. The appropriate US patent was granted in August 2012.

Surface functionalization is an appropriate method for the modification of materials used in medicine. The method has been successfully applied to improve the biocompatibility of vascular grafts made from knitted polymer

A US patent protecting our method for the local functionalization of polymer materials was granted in August 2012.

o improve the biocompatibility of vascular grafts made from knitted polymer fibres. Systematic research showed that insufficient biocompatibility of this material causes the activation of blood platelets and the release of enzymes responsible for triggering thrombotic reactions. The activation of blood platelets could be minimized using reactive particles from oxygen plasma to modify the surface properties of artificial blood vessels. The properly

selected fluxes of both positively charged and neutral radicals allow for a decrease of highly activated forms of blood platelets by well over an order of magnitude, with which the risk for undesired thrombotic reactions is also significantly reduced.

Plasma treatment is also a suitable method for the modification of cellulose materials. The effect of interaction between the plasma radicals and these materials is several-fold. The reactive particles cause total oxidation of impurities that are likely to appear on cellulose. The result of this interaction is the removal of almost all organic



Figure 3: SEM image of a well-activated spread blood platelet

impurities. Next, the treatment by oxygen plasma causes the formation of dangling bonds and functional groups of high polarity. This effect is due to the interaction of hard UV radiation and reactive predominantly neutral oxygen radicals with cellulose materials. Furthermore, oxygen radicals cause controlled inhomogeneous etching of cellulose fibres and thus the formation of nanostructured surfaces. All there effects reflect in excellent adhesion of coatings that are deposited on plasma-treated cellulose in order to modify the surface properties. In fact, the combination of a plasma treatment followed by the deposition of highly hydrophobic thin films by the sol-gel method allows not only for super-hydrophobic properties but also for oleo-phobic and thus self-cleaning properties.

Highly non-equilibrium gaseous plasma created in gases such as oxygen, carbon dioxide and sulphur dioxide is also suitable for the synthesis of metal oxide nanoparticles. Various metals form oxides of different morphology upon exposure to a plasma environment. The hematite nanostructures gain different shapes upon treatment with oxygen plasma with different parameters. The choice of shapes include nano-needles, a dense forest of nano-wires

as well as nano-walls, all depending on fluxes of different particles created in an oxygen plasma onto the surface of substrates. These structures have interesting photochemical properties so they are suitable for manufacturing nanowire array electrodes for water splitting.

The European project PlasmaNice: Atmospheric plasmas for nanoscale industrial surface processing, funded under 7th FP was accomplished successfully. This project lasted for four years and involved 15 European partners

from research organizations and industry. The result of the project is a new technology for the industrial in-line deposition of functional coatings on paper and plastic substrates for packaging assisted by atmospheric plasmas as well as corresponding production line. Our group performed precise surface characterization of plasma deposited sol-gel coatings using the XPS, AFM and ToF-SIMS methods. We determined the correlation between the plasma

parameters, the degree of surface functionalization and the thickness of the deposited coatings. In the frame of the project we also developed a new method for the fast and in-line monitoring of the efficiency of the air plasma surface activation at very high velocity, which has a great potential for industrial applications.

The characterization of surfaces and interfaces, layered structures and nanomaterials requires the application of advanced surface-sensitive analytical techniques. In our department X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES) and atomic force microscopy (AFM) have been used successfully, both for basic research and for the characterization of technological samples. Our research group is recognized worldwide as a leading group in the research field of the depth profiling of thin films and multilavers at a high depth resolution.

A new method, time-of-flight secondary ion mass spectroscopy (ToF-SIMS), has been introduced in our laboratory. It is the only instrument of this type in Slovenia. This advanced method enables a precise characterization of



Figure 4: AFM image of a fully spread blood platelet

the chemical structure of surfaces of organic materials like polymers and biomaterials, as well as a variety of inorganic materials like metals, semiconductors, composites, nanostructure materials, etc. The ToF-SIMS method is based on

the bombardment of a sample with clusters of Bi ions, subsequent desorption of ionized surface molecules and ionized atomic clusters, followed by a mass analysis of the desorbed species. The mass analyser determines the masses of the ions on the basis of the time of flight of ions in a multichannel mode, which allows for fast analyses. The new ToF-SIMS spectrometer operates in

a ultrahigh vacuum and allows for the chemical imaging of solid surfaces with a lateral resolution of 50 nm and mass spectroscopic analysis up to 10,000 mass units with a high mass resolution. The characterization depth is only about 1 nm, which makes this method one of the most surface-sensitive ones. Unlike most other surface-sensitive techniques it is also a suitable technique for a determination of the hydrogen distribution on the sample surface. This new analytical equipment will allow us to follow new trends in the development, treatment and characterization of new materials as well as to synthesize our own advanced materials.

In the field of thin-film physics we continued with a systematic study of interfacial reactions in different multi-layered systems like Al/Ti, Ni/Ti and Si/C composed of 20-50-nm-thick layers and exposed to different activation mechanisms like ion beam mixing, thermal treatment or laser illumination. The applied processing can be interesting for the fabrication of tightly bond multi-layered structures with gradual changes of their composition and properties. Interactions induced in Al/Ti multilayers by the implantation of high-energy Ar⁺ ions were studied by XPS and AES in collaboration with the Institute for Nuclear Sciences from Vinča, Serbia. It was found that ion irradiation induced a progressive intermixing of the multilayer constituents and Al-Ti nanoalloying. The resulting nanocrystalline structure had a graded composition with non-reacted or interdiffused Al and Ti, as well as γ -AlTi and AlTi, intermetallic phases. Most intense reactivity was observed around the mid-depth of the multilayers, where most energy was deposited by the impact ions. Using the XPS spectroscopic method we studied the electronic properties and the ratio of the valence states of Ni3+/Ni2+ in electrochromic coatings deposited from N₁ _O pigment/NiO₂H₂ dispersion in collaboration with National Institute of Chemistry, Ljubljana. These coatings demonstrate a large potential for manufacturing plastic film based electrochromic devices, providing transmitted-light modulation. Lowtemperature curing enabled the deposition of pigment coatings on conducting polymer films.

Our three-chamber UHV system with a quadrupole mass spectrometer was upgraded to allow for very sensitive and quantitative gas analyses. It was applied successfully to measure the gas release from various organic and inorganic materials. The problem of water adsorption and re-adsorption in the UHV system oxidation and electron reduction.

that causes the main inaccuracy was solved by keeping the analytical part of the system at 120°C. The performance has been tested for the quantitative outgassing rate measurement of the water from glass samples kept at various temperatures as well as for newly synthesized organic rigid foams that may be applied in advanced thermal insulations. The new open-pore rigid organic foams that are stable at temperatures up to 200°C were synthesized at the

The activation of blood platelets is reduced dramatically on polymer materials treated by oxygen plasma.

ChemComm



Figure 5: The cover page of the journal Chemical Communications advertises our paper U. Cvelbar et al, Sub-oxideto-metallic uniformly-nanoporous crystalline nanowires by plasma

A new analytical method Secondary Ion Mass Spectroscopy - TOF-SIMS was introduced for the advanced characterization of the surface chemical structure of organic materials.



Figure 6: A new ToF-SIMS spectrometer for the characterization of the chemical structure of organic materials has been installed (left image). It allows for the chemical imaging of surfaces with a lateral resolution of 50 nm and mass spectroscopy analysis up to 10,000 mass units with a high mass resolution. TOF-SIMS images of the chemical composition on the surface of cotton fibres after the deposition of silane-based coatings with F-based species (right).

After four years the EU project PlasmaNice, involving 15 partners, successfully finished with the development of new equipment and technology for the industrial deposition of silane-based functional coatings on paper and plastic packaging materials assisted by atmospheric plasmas.



Figure 7: Industrial pilot line for the treatment of packaging materials like paper and plastics at the Technical University Tampere (TUT) in Finland, where new equipment for the deposition of hybrid silane-based coatings was installed, based on air plasma. Collaboration in the PlasmaNice EU project was coordinated by dr. J. Kovač.

Melamin Company from Kočevje (Slovenia). Using our very sensitive techniques, developed previously, it was revealed that they have an extremely low outgassing rate. Their thermal conductivity equals to 5 mW/(m K) at low pressure. This thermal conductivity was increasing slowly with the pressure of argon up to 10 mbar, which reveals their very small average pore diameter. Since the density of these foams is acceptable at about 50 kg/m³ they are extremely attractive as the core material in vacuum insulating panels (VIP). A literature survey reveals that these foams are the only organic material that is stable inside a VIP for decades. Novel VIP solutions are the most promising approaches to energy-efficient devices and buildings.

Our formerly revealed physical picture that electron field emission from graphite platelets being only a few nanometres thick is responsible for the stable operation of gas surge arresters has been applied and upgraded. By a well-planned series of experiments the breakdown voltage drift with time in gas surge arresters has been explained and stabilized for unipolar or bipolar pulses. By using a proper design of inter-electrode gap, by proper gas mixture and subsequent thermal treatment of the arrester, an extremely stable breakdown voltage was achieved in bipolar breakdown events. Our industrial partner Iskra Zaščite has already launched a new generation of reduced size and stable breakdown voltage gas-surge arresters on the global market. Besides the extremely high stability, the advantage of the new gas surge arrester is a substantially reduced volume compared to competing products.

Some outstanding publications in the past year

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Awards and appointments

1. Dr. Martina Modic; Award for the best Poster at the 14th Joint Vacuum Conference, Poster with title "Shear stress and platelet adhesion on plasma treated polymer surfaces".

Organization of conferences, congresses and meetings

1. IUVSTA Workshop, Cerklje na Gorenjskem, Slovenia, 9-12. 12. 2012

Patents granted

- 1. Miran Mozetič, Alenka Vesel, Uroš Cvelbar, Method and device for local functionalization of polymer materials, US8247039 (B2), United States Patent and Trademark Office, 21.8.2012..
- 2. Gregor Primc, Miran Mozetič, Method for dynamically controlling the density of neutral atoms in a plasma vacuum chamber and a device for the processing of solid materials by using this method, SI23626 (A), Urad RS za intelektualno lastnino, 31.7.2012..
- 3. Rok Zaplotnik, Alenka Vesel, Miran Mozetič, Device for high-frequency gas plasma excitation, SI23611 (A), Urad RS za intelektualno lastnino, 31.7.2012.

INTERNATIONAL PROJECTS

- Development of a vacuum measurement method with respect to vacuum glazing AGC Glass Europe Dr. Vincenc Nemanič
- 7. FP PlasmaNice: Atmospheric plasmas for nanoscale industrial surface processing European Commission Asst. Prof. Janez Kovač
- 7. FP EURATOM: deuterium interation kinetics metals relevant to iter or demo 1.4.4. -FU; Annex 3 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology
- Dr. Vincenc Nemanič
- 7. FP EURATOM: Removal of deposits by neutral oxygen and nitrogen atoms 1.4.2.-FU; Annex 3 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology
- Prof. Miran Mozetič 5. 7. FP - EURATOM, MHEST Association: Application of neutral atoms for fuel removal in
 - gaps; WP11-PWI-02-04-01/PS Ministry of Higher Education, Science and Technology
- Prof. Miran Mozetič
 FP MHEST ASSOCIATION: Investigation of growth of fuzz on tungsten under high heath loads and exposure to hydrogen plasma
- Ministry of Higher Education, Science and Technology Prof. Miran Mozetič
- FP EURATOM, MHEST Association: deuterium retention and release from metal surfaces - 1.4.4-FU Ministry of Education, Science and Sport
 - Dr. Vincenc Nemanič
- FP EURATOM, MHEST Association: Extending knowledgebase on fuel release (and retention) of Be-containing mixed materials; WP12-IPH-A01-3-04/PS-1 Ministry of Education, Science and Sport Dr. Vincenc Nemanič
- 9. COST MP1101: Biomedical applications of atmospheric pressure plasma technology COST Office
 - Asst. Prof. Uroš Cvelbar
- NATO Planning Grant; SfP 984555: Atmospheric pressure plasma jet for neutralisation of CBW (Chemical Biological Weapons) NATO
 - Asst. Prof. Uroš Cvelbar
- 11. Thermoionic energy conversion Public Research Agency Dr. Vincenc Nemanič
- Nanowires for photoelectrochemical energy conversion and water splitting Public Research Agency
- Asst. Prof. Uroš Cvelbar 13. Plasma synthesis and application of nanowalls
- Public Research Agency Asst. Prof. Uroš Cvelbar
- Plasma synthesis and deposition of quantum dots Public Research Agency
- Asst. Prof. Uroš Cvelbar
- Determination of interdiffusion coefficients in nano-layered structures by high resolution Depth Profiling Public Research Agency
 - Asst. Prof. Janez Kovač
- 16. Plasma diagnostics for applied research of dusty plasmas with nanoparticles Public Research Agency
- Asst. Prof. Uroš Cvelbar 17. Plasma treatment of titanium stents Public Research Agency
- Asst. Prof. Uroš Cvelbar 18. Investigation of microwave disc
- Investigation of microwave discharges applicable in biomedicine and nanotechnology Public Research Agency Prof. Miran Mozetič
- Plasma-assisted Synthesis of nano-objects Public Research Agency Asst. Prof. Uroš Cvelbar

- 20. Formation of nanocomposite thin films in dusty magnetized plasma Public Research Agency Asst. Prof. Alenka Vesel
- Hydrogen interaction with W/Be films relevant for fusion reactors Public Research Agency Dr. Vincenc Nemanič

RESEARCH PROGRAMS

- 1. Vacuum technique and materials for electronics Dr. Vincenc Nemanič
- Thin film structures and plasma surface engineering Prof. Miran Mozetič

R & D GRANTS AND CONTRACTS

- 1. Use of nanoparticles as additives in lubricants and in tribology Asst. Prof. Janez Kovač
- Near-net shape nanoparticle-reinforced polymer-composites for highly-loaded advanced mechanical components with superior tribological performance Asst. Prof. Janez Kovač
- 3. Organic-inorganic thin film structures for electronics components Asst. Prof. Janez Kovač
- 4. Multifunkctional nanocomposite coatings and paints Asst. Prof. Janez Kovač
- Research and development of integrated overvoltage protection devices based on gaseous discharger toward a reliable miniature technical solution Dr. Vincenc Nemanič
- Development of advanced processes for attending high efficient nano modified textile materials Prof. Miran Mozetič
- Synthesis and functionalization of composite nanobeads for early diagnosis of neurodegenerative diseases
 Asst. Prof. Alenka Vesel
- Superhydrophilicity of surfaces and its application in technological processes for industrial application Asst. Prof. Uroš Cvelbar
- Ignition and self-extinguishing of arc in a gas surge arrester at high overvoltages Dr. Vincenc Nemanič
- Plasma treatment of vascular grafts Prof. Miran Mozetič
- Multifunctional anostructured films for artificial implants corrosion and tribocorrosion processes
- Asst. Prof. Janez Kovač 12. Synthesis of nanowires for regenerative energy cells Asst. Prof. Uroš Cvelbar
- Colour, absorption and protective nanolayer coatings for aluminium alloy Asst. Prof. Janez Kovač
- Functionalization of biomedical samples by thermodynamic non-equilibrium gaseous plasma Prof. Miran Mozetič
- Toward ecologically benign alternative for cleaning of delicate biomedical instruments Asst. Prof. Alenka Vesel
- 16. Preparation of hemocompatible polymeric surfaces for biomedical applications Dr. Ita Junkar
- 17. Biopackaging, EUREKA: Development of bioactive packaging Prof. Miran Mozetič

NEW CONTRACTS

 Nanowire synthesis for regenerative energy cells Kolektor Group, d.o.o. Asst. Prof. Uroš Cvelbar



- Functionalization of biomedical samples by thermodynamically non-equilibrium gaseous plasma **BIA Separations** Prof. Miran Mozetič
- VISITORS FROM ABROAD
- 1. Prof. Satomi Tajima, Nagoya University, Japan, 19.-24. 2. 2012
- Prof. Hitoshi Watanabe, Nagoya University, Japan, 19.–24. 2. 2012 Prof. Kostyantyn Ostrikov, CSIRO, Sydney, Australia, 16. 4.–22. 7. 2012 2.
- 3.
- Dr. Tonči Tadič, Rudjer Bošković Institute, Zagreb, Croatia, 24. 4. 2012 Dr. Nikola Radič, Rudjer Bošković Institute, Zagreb, Croatia, 24. 4. 2012
- 5. Dr. Hans Georg Cramer, ION TOF, Münster, Germany, 7.-18. 5. 2012 6.
- Paul Brunet, University of Toulouse, Toulouse, France, 14.-20. 5. 2012
- Dr. Davor Peruško, Vinča Institute of Nuclear Science, Belgrade, Serbia, 20.-26. 5. 2012 8.
- Prof. Sabu Thomas, Mahatma Gandhi University, Kottayam, Kerala, India, 30.-31. 5. 2012 9.
- 10. Dr. Kinga Kutasi, Research Institute for Solid State Physics, Budapest, Hungary, 1.-7. 7. 2012
- 11. Dr. Francisco L. Tabares Vazques, CIEMAT, Madrid, Spain, 13.-22. 8. 2012
- 12. Daniel Alegre, CIEMAT, Madrid, Spain, 19. 8.-9. 9. 2012
- 13. Cedric Labay, University of Barcelona, Barcelona, Spain, 8.-23. 9. 2012
- 14. Dr. Richard Clergereaux, University Paul Sabatier, Toulouse, France, 22.-27. 10. 2012
- STAFF

Researchers

- Asst. Prof. Uroš Cvelbar
- Asst. Prof. Janez Kovač
- 3. Prof. Miran Mozetič, Head
- Dr. Vincenc Nemanič 4.
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- 10. Dr. Martina Modic
- 11. Dr. Rok Zaplotnik
- Postgraduates
- 12. Gregor Filipič, B. Sc.

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- 4. Lenka Chvátalova, Roman Čermak, Aleš Mraček, Ondrej Grulich, Alenka Vesel, Petr Ponížil, Antonín Minařík, Uroš Cvelbar, Lubomír Beníček, Petr Sajdl, "The effect of plasma treatment on structure and properties of poly(1-butene) surface", Eur. Polym. J., vol. 48, no. 4, pp. 866-874, 2012.
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- 15. Dr. Cristian P. Lungu, National Institute for Laser, Plasma and Radiation Physics, Bucharest, Romania, 5.-9. 11. 2012
- 16. Dr. Corneliu Porosnicu, National Institute for Laser, Plasma and Radiation Physics, Bucharest, Romania, 5.-9. 11. 2012
- Dr. Sanghoo Park, KAIST, Daejeon, Republic of Korea, 2.-13. 12. 2012
- 18. Dr. Kinga Kutasi, Research Institute for Solid State Physics, Budapest, Hungary, 5.-13. 12. 2012
- 19. Prof. Masaru Hori, Nagoya University, Nagoya, Japan, 5.-13. 12. 2012
- 20. Prof. Wonhoe Choe, KAIST, Daejeon, Republic of Korea, 9.-13. 12. 2012
- 21. Prof. David Ruzic, University of Illinois at Urbana-Champain, USA, 12.-13. 12. 2012
- Dr. Sanja Medenica, Institute for public health of Montenegro, Podgorica, Montenegro, 22. 17.-24.12.2012
- 23. Dr. Danijela Vujošević, Institute for Public Health of Montenegro, Podgorica, Montenegro, 17.-24. 12. 2012
- 13. Gregor Jakša, B. Sc.
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- Urška Kisovec, B. Sc. 22.
- 23. Janez Trtnik

** postgraduate financed by industry

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INDEPENDENT SCIENTIFIC COMPONENT PART OR A

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PATENT APPLICATION

- 1. Miran Mozetič, Gregor Primc, *Method for dynamically controlling the density of neutral atoms in a plasma vacuum chamber and a device for the processing of solid materials by using this method*, W02012099547 (A1), World Intellectual Property Organization, 26.7.2012.
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PATENT

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MENTORING

- Kristina Eleršič, Superhydrophility of plasma treated materials: doctoral dissertation, Ljubljana, 2012 (mentor Miran Mozetič; comentor Uroš Cvelbar).
- Martina Modic, Hemostatic response of plasma treated artificial grafts: doctoral dissertation, Ljubljana, 2012 (mentor Miran Mozetič; comentor Rok Kostanjšek).
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DEPARTMENT OF SOLID STATE PHYSICS

Our research program is focused on the study of the structure and dynamics of disordered and partially ordered condensed matter at the atomic and molecular levels with a special emphasis on phase transitions. The purpose of these investigations is to discover the basic laws of physics governing the behaviour of these systems, which represent the link between perfectly ordered crystals, on the one hand, and amorphous matter, soft condensed matter and living systems, on the other. Such knowledge provides the key to our understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of new multifunctional materials, nanomaterials and biomaterials for new applications. An important part of the research program is devoted to the development of new experimental methods and techniques in the field of magnetic resonance, magnetic resonance imaging, fluorescence microspectroscopy, scanning tunnelling, electronic and atomic force microscopy, as well as dielectric relaxation spectroscopy and dynamic specific-heat measurements.

The experimental techniques used are:

- One-(1D) and two-dimensional (2D) nuclear magnetic resonance (NMR) and relaxation, as well as quadrupole (NQR) resonance and relaxation,
- Multi-frequency NMR in superconducting magnets of 2 T, 6 T and 9 T, as well as the dispersion of the spin-lattice relaxation time T_1 via field cycling,
- Nuclear double resonance and quadrupole double resonance such as ¹⁷O-H and ¹⁴N-H,
- Fast field cycling NMR relaxometry,
- Frequency-dependent electron paramagnetic resonance (EPR) and 1D and 2D pulsed EPR and relaxation,
- MR imaging and micro-imaging, _
- Measurement of the electronic transport properties,
- Magnetic measurements,
- Fluorescence microscopy and microspectroscopy,
- Linear and non-linear dielectric spectroscopy in the range 10⁻² Hz to 10⁹ Hz,
- Electron microscopy and scanning tunnelling microscopy,
- Atomic force microscopy and force spectroscopy, _
- Dynamic specific heat measurements.

The research program of the Department of Solid State Physics at the "Jožef Stefan" Institute is performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the J. Stefan International Postgraduate School. In 2012, the research was performed within three research programs:

- Magnetic resonance and dielectric spectroscopy of smart new materials
- Physics of Soft Matter, Surfaces and Nanostructures
- Experimental Biophysics of Complex Systems

I. Research programme "Magnetic resonance and dielectric spectroscopy of smart new materials"

In 2012 the members of the program group published 55 original scientific papers in international peer-reviewed scientific journals. Several articles were published in high-impact journals (one article in Nature Photonics, one in Chemical Society Reviews and four articles in Phys. Rev. Letters. The investigations were focused on the following research fields.

Quasicrystals and complex metallic alloys

We have determined the anisotropic physical properties of decagonal quasicrystal d-Al-Co-Ni along three directions in the quasi-periodic plane and demonstrated the anisotropy of the transport coefficients (electrical resistivity, thermoelectric (Q) and along the 10-fold periodic direction (10).

300 250 10 (moΩu) 2 200 150 2' bis σ 100 10 50 0 150 200 250 300 350 50 100 0 T (K) 1.00 0 0.95 b) ¥0.90 ő, 0.85 10 0.80 0.75 50 100 150 200 250 300 350 ò T (K)

Figure 1: Anisotropic electrical resistivity of a decagonal quasicrystal d-Al-Co-Ni, measured

Head: Prof. Igor Muševič





F-5

The group has investigated important open issues in the electronic properties of quasicrystals and complex metallic alloys, quantum magnetism in low-dimensional spin systems, critical properties of nanostructures, physical properties of materials with giant electrocaloric and thermoelastic effects, new metallic materials for hydrogen storage and developed novel pharmaceutical and biological substances. The group has also developed a novel spectroscopic method utilizing polarized X-rays on the nanometric scale.



Figure 2: Characteristic temperature-dependent electrical resistivity and thermoelectric power of icosahedral quasicrystals, exhibiting a pseudogap in the electronic density of states at the Fermi energy.

power, Hall coefficient and thermal conductivity) and magnetic susceptibility between the quasi-periodic plane and the periodic 10-fold direction. In contrast, no anisotropy was found within the quasi-periodic plane (Figure 1.).

J. Dolinšek was invited by the Editors of the Chemical Society Reviews to write a review paper on the electrical and thermal transport properties of icosahedral and decagonal quasicrystals (Figure 2). This review paper summarized the current state of the art in the field of physical properties of icosahedral and decagonal quasicrystals, giving a survey of the experimental results and theoretical models. A large part of the paper is based on the results obtained in the author's laboratory at the J. Stefan Institute.

Quantum magnetism

By means of NMR spin-lattice relaxation time, we have studied the spin dynamics as a function of the magnetic field in two quasi-one-dimensional quantum antiferromagnets: the anisotropic spin-chain system NiCl_2 4SC(NH₂)₂ and the spin-ladder system (C₅H₁₂N)₂CuBr₄. We confirmed that the spin excitations in both systems evolve from magnons to spinons when crossing the critical field, in accordance with theoretical predictions. In the vicinity of the critical field, we showed that spin excitations are neither magnons nor spinons, while the spin dynamics scales in accordance with quantum criticality. We showed that the behaviour in both systems is equivalent, thus demonstrating the universality of quantum-critical behaviour. The work was published in *Phys. Rev. Lett.*, see Figure 3.

Members of our department together with a group of international collaborators investigated the ground state of the geometrically frustrated system FeTe₂O₅Br, which is characterized by low-temperature multiferroicity. We have shown that the emergence of an incommensurate amplitude-modulated magnetic structure depends on the magnetic frustration that originates from the topology of this particular spin system. Surprisingly, the system is in fact characterized by magnetic chains, which are coupled by frustrated exchange interactions. The same group of authors investigated

the stability of the incommensurate magnetic ordering at the lowest experimentally accessible temperatures using neutron diffraction measurements at 53 mK. Muon spin relaxation measurements have revealed that in spite of long-range ordering the spin dynamics does not freeze even in the limit of $T \rightarrow 0$ (Figure 4). The amplitude-modulated magnetic structures serve as a model system for the coexistence of long-range order and persistent spin dynamics. A layered Kagome-like Cu₃Bi(SeO₃)₂O₂Br compound was studied using neutron diffraction, bulk magnetization and magnetic susceptibility measurements. At $T_{N} = 27.4$ K a transition into the long-range antiferromagnetic



Figure 3: Characteristic phase diagram of a one-dimensional quantum antiferromagnet around the critical field Bc1 contains three phases with different spin excitations: with magnons (gapped), with spinons (TLL) and intermediate quantum critical region.

ordered phase occurred. The magnetic structure is composed of alternating ferrimagnetic *ab* layers, with the Cu²⁺ (*S*=1/2) magnetic moments slightly canted away from the *c* axis. This magnetic structure was ascribed to the competition between ferro- and antiferro-magnetic interactions within the *ab* layers and additional weak antiferromagnetic interlayer interactions. When the magnetic field perpendicular to the layers exceeds $B_c = 0.8$ T, a metamagnetic transition occurs, where every second layer flips (Figure 5). In combination with other techniques we were able to estimate the strength of individual Cu-...-Cu exchange interactions.

Spectroscopy with polarized X-rays at the nanoscale

Near-edge X-ray absorption spectroscopy (NEXAFS) is an essential analytical tool in material science. Combining NEXAFS with scanning transmission X-ray microscopy (STXM) adds spatial resolution and the possibility to study individual nanostructures. In an article published in *Nature Photonics*, we described a full-field transmission X-ray microscope (TXM) that generates high-resolution, large-area NEXAFS data with a col-

lection rate two orders of magnitude faster than is possible with STXM (Figure 6). We present image stacks and polarization-dependent NEXAFS spectra from individual anisotropic sodium and protonated titanate nanoribbons ((Na,H)TiNRs, HTiNRs)). The combined NEXAFS-TXM technique has the advantage that one image stack visualizes

a large number of nanostructures and therefore already contains statistical information. This new high-resolution NEXAFS-TXM technique opens the way to advanced nanoscale science studies.

Study of the critical properties of nanostructured materials and materials with large electrocaloric and thermomechanical effects

We showed that the refrigerant capacity of PLZT ceramics and ferroelectric polymer films exceed several times all previously known materials, including the magnetocaloric materials. By using high-resolution calorimetry we proved the existence of the phase transition line between the glassy and ferroelectric phase of relaxor ferroelectrics (Figure 7) and explained the anisotropy of criticality in these systems. We described the way to control the temperature profile of the thermomechanical response in liquid-crystal elastomers via different physical parameters such as mechanical fields and the state of the order during the crosslinking procedure. We showed that highly confined liquid crystals exhibit a crossover in the dimensionality of the problem.

Relaxor polymers and ceramic materials

In collaboration with researchers from the Pennsylvania State University, USA, the electrically-induced behaviour was compared in a non-stretched

and uniaxially stretched P(VDF-TrFE-CFE) terpolymer - a member of the relaxor polymer family that exhibits fast response speeds, giant electrostriction, high electric energy density, and a large electrocaloric effect. Substantial differences in the dielectric response, polarization, electrocaloric response, and induced electrostrictive strain of the non-stretched and stretched terpolymer were detected and explained. The results suggest that the electrically-induced properties of relaxor polymer films can be tailored by controlling the preparation conditions. In collaboration with researchers from Nanjing University, China, we have reported on the structural, thermal, and dielectric properties of relaxor P(VDF)-based terpolymer/copolymer blends on aluminum foil, i.e., the first relaxor polymer blends developed on a metal surface. The detected response has been explained by calculations that take into account the fact that two similar dynamic processes (relaxor dynamics in the crystalline regions and a glassy transition in the amorphous matrix) superimpose in the same temperature range (Figure 8).

The dielectric response of core-shell structured ceramic materials (composed of semiconducting grains separated by insulating grain boundaries) has been modelled in terms of an equivalent electric circuit with elements that describe distinctive contributions of grains and grain boundaries. By taking into account a proper temperature dependence of the individual elements of the circuit, the temperature- and frequency-dependent dispersive dielectric behaviour, typically observed in these materials, has been obtained. The modelling results have been applied to the experimentally detected dielectric response of CaCu₃Ti₄O₁₂ thin films that exhibit, for a ceramic thin film, extremely high values of the dielectric constant. In addition, the influence of parasitic inductance and the resistance of the experimental setup on the measured dielectric response was calculated. A novel experimental setup has been installed in 2012 that enables a simultaneous detection of the electrical (four-point electrical conductivity) and thermoelectrical (thermoelectric voltage, the Seebeck coefficient) properties from room temperature up to 1000°C.

Hydrogen-storage metallic alloys

The crystal structure, bonding and magnetic changes upon hydrogenation of TiFe_{1.v}Ni_v alloys Figure 5: Magnetic structure in Cu₃Bi(SeO₃)₂O₃Br with different hydrogen and Ni contents were investigated (Figure 9). In crystalline samples, a system (a) in the absence of external magnetic reversible second-order phase transition from the α -phase (with soluble hydrogen) through a *field and* (b) in field of 1 *Tesla applied along the* mixture of α - and β -phase into a pure β -phase was found. In amorphous samples, no transition c axis. The different colours of the arrows denote the magnetic state of α - and β -phase into a pure β -phase was found. In amorphous samples, no transition d are the magnetic state of α - and β -phase into a pure β -phase was found. In amorphous samples, no transition d are the magnetic state of α - and β -phase into a pure β -phase was found. In amorphous samples, no transition d are the magnetic state of α - and β -phase into a pure β -phase was found. In amorphous samples, no transition d are the different colours of the arrows denote the magnetic state of α - and β -phase into a pure β -phase was found. In amorphous samples, no transition d are the different colours of the arrows denote the different colours of the d was found. The saturation magnetization of the samples increases with hydrogenation and further increases upon hydrogen desorption. The increase of the Ni/Fe ratio in the TiFe, Ni, is found to

result in an increase of hydride cohesive energies and in the systematic shifting of the Fermi energy to lower values, in both pure intermetallics and appropriate hydrides. The hydrogen desorption temperature rises but the maximum amount of hydrogen absorbed under the same conditions decreases. Among the studied materials, TiFe_{0s}Ni₀, was found to be the most promising composition for hydrogen storage.



Figure 4: Decay of muon polarization in FeTe₂O₅Br due to (a) nuclear and (c) electronic magnetic fields. The latter are characterized by their broad distributions (in the inset), which originate from an amplitudemodulated magnetic ground state. (b) Calculated electrostatic potential within the crystallographic unit cell.



the magnetic moments at two crystallographically inequivalent Cu sites.



Figure 6: Workflow for NEXAFSTXM measurements. a) X-ray optical set-up of the TXM for NEXAFS studies. Monochromatized radiation from the undulator is focused by a reflective capillary condenser into the object field. A zone plate objective forms a magnified image. By choosing regions of interest (ROIs), the optical density can be calculated for each ROI using the sample-free region in its vicinity. As many nanostructures are within the field of view, one photon energy stack contains statistical information. b) Stack of (Na,H)TiNR images recorded at different energies. The NEXAFS spectrum is recorded on a ROI. c) Scheme showing a ROI for recoding the transmitted photon flux (1) and incident photon flux (I_o).



Figure 7: Electric-field-temperature phase diagram of the PMN [110] relaxor ferroelectric.



Figure 8: Dielectric response of the P(VDF-TrFE-CFE) terpolymer film and its blends with P(VDF-CTFE) copolymer on aluminium foil – the first relaxor polymer blends, developed on a metal surface.

Mechanochemical synthesis, elastomers and liquid crystals

Using quadrupole-perturbed nuclear magnetic resonance of ²³Na, we monitored the chemical processes governing the mechanochemical synthesis of NaNbO₃. The results reveal the existence of a transitional amorphous carbonato complex with an atypical Nb-O bond. We successfully detected ¹⁴N quadrupole-perturbed nuclear magnetic resonance in photoisomerizable nematogen 7AB, in spite of extremely short spin-lattice relaxation times, typically about 10 us, which combined with a large quadrupole coupling constant normally inhibit the detection of resonance. In the specific case of 7AB, a relatively small and well-resolved 14N quadrupole doublet can nevertheless be detected, since the N=N bond exhibits reorientations about the long molecular axis at the angle close to the magic angle. Taking into account the differences in the temperature dependence of ²H and ¹⁴N doublet splittings, we also determined the temperature dependence of the molecular biaxiality. The temperature-concentration (T-f) phase diagram of the binary confined liquid crystal 7AB was also determined (Figure 10). The non-equilibrium concentration of cis-isomers, f, was controlled by illumination with UV light. The establishment of the equilibrium state with all trans-isomers was monitored in-situ via the quadrupole-perturbed nuclear magnetic resonance of ²H. Isotropic-nematic phase coexistence regions were determined by analysing the time-dependences of the spectra. This work was published in Physical Review Letters.

Ferroelectrics, hydrogen-bonded systems, pharmaceutical and biological substances

We investigated organic ferroelectrics, hydrogen bonds, pharmaceutical and biological substances, cocrystals and crystal polymorphs. Phase transitions in a metal-organic perovskite with an azetidinium cation, which exhibits giant polarizability, were investigated using differential scanning calorimetry (DSC) and ¹H nuclear magnetic resonance (NMR) measurements. The DSC results indicated successive phase transitions at 254 and 299 K. The temperature dependence of the spin–lattice relaxation time T_1 determined by NMR indicated that the activation energy for cation ringpuckering motion was 25 kJ mol⁻¹ in phase I (T > 299 K).

The ¹⁷O NQR frequencies have been measured in ciscyclobutane-1,2dicarboxylic acid and the quadrupole coupling tensors have been determined at various temperatures. The temperature dependence of the ¹⁷O quadrupole coupling tensors at the ¹⁷O···H-O oxygen positions was analysed in the model of proton exchange and the energy differences of the two proton configurations obtained by this analysis agree with the values obtained from the O-H distances. The model shows that the population of an oxygen lone pair orbital is at this oxygen position reduced from 2 to approximately 1.3.

The stability of the antihypertensive drug nifedipine (NIF) has been studied in the solid state by ¹H-¹⁴N NMR-NQR double resonance (NQDR) and theoretically by the Density Functional Theory (DFT). The photoconversion of NIF to NO-NIF in the solid was found to be accompanied with the electron density redistribution at nitrogen sites (-NH- to -N= and $-NO_2$ to -NO) and proved to be successfully detected with the identification of photoproducts by ¹H-¹⁴N NQDR and DFT methods. A potential anti-leukemic and anti-cancer agent, 2-thiocytosine (2-TC), has been studied experimentally in the solid state by ¹H-¹⁴N NMR-NQR double resonance (NQDR) and theoretically by the quantum theory of atoms in molecules (QTAIM)/density functional theory (DFT). Eighteen resonance frequencies on ¹⁴N were detected at 180 K and assigned to particular nitrogen sites ($-NH_2$, -N=, and -NH-) in 2-thiocytosine. This study demonstrates the advantages of combining NQDR and DFT to extract detailed information on the H-bonding properties of crystals with

complex H-bonding networks. Solid-state properties were found to have a profound impact on the stabilities and reactivities of both compounds.

Nuclear quadrupole resonance (NQR) was used as a method for the characterization of cocrystals and crystal polymorphs. 14N NQR spectra of several cocrystals of carbamazepine have been measured together with the 14N NQR spectra of cocrystal formers. The results show that the ¹⁴N NQR spectrum of a cocrystal and the ¹⁴N NQR spectra of cocrystal formers differ well outside the experimental resolution. It is further described how the NQDR techniques, that have been used to measure the ¹⁴N NQR frequencies, can be used to check the homogeneity of a polycrystalline sample and to monitor the stability of a metastable crystal polymorph.

Nitrogen atoms are present in a number of solid explosives and illicit substances. The nuclear quadrupole resonance (NQR) spectra and spin-lattice relaxation of the nitrogen atomic nucleus ¹⁴N can be used to characterize these compounds and to distinguish between possible crystal polymorphs. After the characteristic ¹⁴N NQR frequencies and spin-lattice relaxation rates in a compound are determined, NQR can be used to detect these compounds and, in the case of crystal polymorphs, also to determine the method of preparation. The 14N NQR frequencies and spin-lattice relaxation rates are measured either by pulse NQR or by nuclear quadrupole double resonance Figure 9: TiFe_{0.5}Ni_{0.5} supercell

TiFe0.50Ni0.50



II. Research programme "Physics of Soft Matter, Surfaces and Nanostructures"

The investigations of the research program "Physics of Soft Matter, Surfaces and Nanostructures" are focused on novel complex soft matter systems and surfaces with specific functional properties. We investigated in particular liquid-crystalline elastomers and dendrimers as novel multifunctional materials, nematic colloids, molecular motors,

soft-matter photonic crystals and novel synthetic or self-assembled micro- and nano-structures. The aim of the program is to understand the structural and dynamical properties of these systems, their interactions, their function at the molecular level, and self-assembly mechanisms in soft matter. The underlying idea is that it is possible to understand complex mechanisms, such as self-assembly, on a macroscopic level, using a simplified physical picture and models. In order to provide a comprehensive approach to the problem, the program combines both experimental and theoretical investigations, supported by modelling and simulations. Special emphasis is given to the possible electro-optic and medical applications.

(NQDR) based on magnetic field cycling.

We have investigated the topology of chiral nematic braids, the optical imprinting of topological defects, the self-assembly of nematic colloids and have found optimal shapes of microswimmers, mimicking simple micro-organisms in Nature. We have demonstrated the excellent tribological properties of MoS, nanoparticles and have demonstrated the first FET transistor based on 2D crystal WS_a.

Modelling of the laser imprinting of defects in nematics

We showed that using Laguerre-Gaussian optical beams, complex structures of typically even higher complexity can be induced in nematics. The role of the absorption - in the bulk or at the surfaces - is addressed, demonstrating complex local heating of the nematic material within the optical beams. Finally, the structures imprinted by

complex optical beams can be good candidates for various further-tuned structures affected by confinement, complex surface anchoring profiles, chirality of nematic, and incorporation into nematic colloids. The work was published in Soft Matter.

Rewiring of nematic braids in chiral nematic colloids

We studied chiral colloidal dimers on the theoretical and experimental level. The influence of the chirality on the tangles in the formalism of tetrahedral rotations is of vital importance if the formalism is to be used to predict the possible structures. Systems with sufficiently complex boundary conditions can assume a large number of metastable configurations. Accurate prediction and the guided simulation of complex structures can accompany the experimental results for chiral defect systems induced optically, by colloidal inclusions, or by confinement. The work was published in Soft Matter. Figure 10: Isonematic lines of photo-isomerized 7AB.



Modelling of cholesteric droplets

We addressed systems of cholesteric liquid-crystal droplets, where the relation between the confinement via the spherical surface of the droplet and the chiral twisting of the liquid crystalline orientational order is specifically expressed. Multiple anisotropic optical profiles are demonstrated, emerging as a result of geometrical confinement.

(a)



Figure 11. Schematic presentation of complex laser induced defects in a nematic

Figure 12. Colloidal dimer in a chiral nematic: Disclination lines and

a 180-degree twist cell is shown. For the C site all three configurations of

four tetrahedral sites where the rewiring of disclinations is possible in

Also, the authors show that changing the intrinsic twisting of the molecular optical axes induces remarkable changes in the droplet structure, modifying the optical and photonic properties of the droplets. The demonstrated approach could be used as a possible mechanism to envisage soft-matter optic and photonic elements in all-photonics circuits. The work was published in *Soft Matter*.

Shape-tuning the colloidal assemblies in nematics

Using numerical modelling, we demonstrate two-dimensional self-assembly of triangular, square, and pentagonal submicrometer-sized platelets in thin layers of nematic liquid crystals. Platelets are decorated with disclinations leading to effective elastic dipoles or quadrupoles. Colloidal assemblies of chains of such elastic dipoles into periodic lattices are formed via diverse rotational and translational shifts to minimize the distortions in the surrounding nematic medium. The work was published in *Soft Matter*.

Elastic anisotropy driven nematic shell restructuring

Confining a nematic liquid crystal to spherical shells with planar degenerate surfaces gives rise to various defect configurations with the total topological charge +2. In eccentric

shells all four disclinations with winding number -1/2 are positioned in the thinner region to minimize their length. By chemically functionalizing these defects one could fabricate colloids with tunable valence. The elastic constant anisotropy, which is experimentally controlled by varying the temperature, leads to a gradual change of defect positions in a notably asymmetric way. On the other hand, when the eccentricity of the shells is changed, the defects increase their separation in a roughly symmetrical way. Controlling the directional-binding capabilities of shells provides a possible route towards the controlled self-assembly of colloids for optical and photonic applications. The research was performed in collaboration with the group in Montpellier.

Dimensional crossover in nano-confined liquid crystals

On decreasing a characteristic confinement length of confined thermotropic liquid crystals (LCs) the role of wetting-surface interactions is gaining in importance due to increasing surface-to-volume ratio. In particular, if noncritical surface interaction exhibits a linear dependence on the order parameter it can erase the phase transition at a critical confinement length. We were the first to demonstrate, theoretically and experimentally, that a different scenario might appear in nanoconfined LCs in the case of relatively weak wetting interactions. Namely, with a decreasing confinement scale the

effective dimensionality of the system is reduced and consequently, the 1st-order phase transition into an orientationally ordered phase is, due to symmetry reasons, replaced by the 2nd-order phase transition. We realized experimentally weak wetting conditions by exploiting memory effects and using relatively flexible LC molecules (12CB). The results were published in *Soft Matter*.



disclinations are shown.

Figure 13. Soft Matter cover page: Modeling of radial defects in cholesteric droplets

Theoretical investigations of artificial swimmers.

We investigated the energetic efficiency of low Reynolds number swimmers driven by self-propulsion along their surface. An example of such swimmers are ciliated protozoa, but also artificial chemiphoretic swimmers. It turns out that the cost of propulsion is proportional to the square of the fluid velocity above the surface, integrated over the surface of the swimmer. We thus determined the swimmer shapes and their velocity distribution in a way that they achieve a given swimming velocity with minimum dissipation while keeping the volume constant. The result is surprising as the optimal shape can, depending on the allowed curvature, contain protrusions along the symmetry axis (Fig. 16 a). The calculated optimal swimmer shapes also show a high degree of similarity with various microorganisms found in nature (Fig. 16 b). The work was published by A. Vilfan in *Phys. Rev. Lett*.

Vapour-trace detection of explosives using chemically functionalized COMB microsensors.

In collaboration with the Faculty of Electric Engineering and the Faculty of Chemistry and Chemical Technology of the University of Ljubljana we have developed and tested a miniature system for the detection of very small concentrations of vapours of various explosives in the atmosphere. The system is based on a very
sensitive microcircuit that uses planar COMB capacitors produced in CMOS technology. The vapour traces of explosives, which are always present in the vicinity of explosive devices, are selectively adsorbed on the electrodes of micro-capacitors that have been previously chemically functionalized with receptor molecules. This change in the capacity of the chemically functionalize capacitor is detected with the sensitivity in the range of an attofarad. We have succeeded in detecting 2 molecules of TNT in 10^{-12} molecules of the carrier gas N₂ (Figure 17).

Friction reduction via single ${\rm MoS}_2$ "mama"-tubes and single ${\rm MoS}_2$ fullerene-like particles

For the first time the coefficients of friction between a silicon AFM tip and a single MoS_2 nanotube or a single MoS_2 nano-onion were found to be much below the values obtained for a flat MoS_2 single crystal or graphite. We revealed a non-trivial dependency of the coefficient of friction on the interaction strength between the nanotube and the underlying substrate that is explained with the dissipation of energy and shear deformation. The MoS_2 nanotubes with a high interaction strength revealed up to four times larger coefficient of friction 0.08 than weakly supported tubes. The results explain the phenomena of the higher friction found for intra-crystalline slip than for inter-crystalline slip. This phenomenon, which is in contradiction with commonly accepted models, was published a quarter of century ago and remained without confirmation until now. We also evidenced that a rolling mechanism of MoS_2 fullerene-like nano-onions is indeed possible at low loads in accordance with recent predictions. The work was published *Nanoscale Research Letters*.

The addition of the MoS_2 nanotubes to the synthetic Polyalphaolefin (PAO) oil significantly improved the friction and wear behaviour in the boundary-lubrication conditions between AISI 52100/DIN 100Cr6 steel counterparts. The coefficient of friction was decreased by more than 2 times, while the wear was reduced by as much as 5–9 times. The use of nanotubes almost completely eliminated any abrasion or deformation of the surfaces in the studied time span. The investigation showed that the formation of a MoS_2 - nanotubes-based tribofilm in the contact area was of key importance for the reduction of friction and wear.

${\rm MoS}_{\rm 2}$ nanotubes mediated polymer melt-processing for novel nanocomposites materials

The MoS_2 nanotubes were introduced into an isotactic polypropylene (iPP) polymer matrix to generate novel nanocomposite materials through an advantageous melt-processing route. The incorporation of INT-MoS₂ generated notable performance enhancements through reinforcement effects, highly efficient nucleation activity, and excellent lubricating ability in comparison with other nanoparticle fillers. The thermal stability of nanocomposites filled with 1 wt.% of INT-MoS₂ was almost 60°C higher than that of neat iPP, the coefficient of friction decreased by 15% and wear by more than 50%.

Chemically synthetized field-effect transistor (FET)

We report the realization of FETs made with a chemically synthesized, layered 2D semiconductor crystal of WS₂. The 2D Schottky-barrier FETs demonstrated ambipolar behaviour and a high $(\sim 10^5 x)$ on/off ratio at room temperature with current saturation. The behaviour was attributed to the

Figure 14. Colloidal platelets in the nematic layer: Two-dimensional clusters of pentagons (a,b) and (c) a stable two-dimensional pentagonal tiling formed after free-energy minimization. Inset shows the binding potential of the tiling as a function of the lattice constants X and Y.



Figure 15. Effect of elastic constant anisotropy on the position of defects in a nematic shell where spherical surfaces are not concentric.



Figure 16: (a) The calculated optimal swimmer shapes for different values of maximum surface curvature. (b) Shapes of three ciliated microorganisms.

presence of an energy bandgap in the 2D crystal material. The FETs show clear photoresponse to visible light. The promising electronic and optical characteristics of the devices combined with the layered 2D crystal flexibility make WS₂ attractive for future electronic and optical devices. This work was published in *Applied Physics Letters*.



Figure 17. The diagram shows the vapour pressure of different explosives as a function of their molecular weight. The detection levels of different noses are presented as well, together with the detection level presently achieved with COMB microcapacitors. This work was published in IEEE Sensors Journal.



Figure 18. (a) AFM image of the topography of MoS₂ nanotubes with a diameter of 170 nm. The scanning force was 3 nN, the scanning region is indicated with the square. (b) Friction force for different directions of scanning along the nanotube.



Figure 19. Optical micrographs of wear traces left on a steel disc after 100 m of sliding of a steel ball. The ball was lubricated with (a) pure PAO base oil, whereas in (b), 5 wt.% of MoS₂ nanotubes have been added to the lubricating oil.

Ultra-cold atoms

A dedicated laboratory for sensitive experiments with ultra-cold atoms is being set up with the first equipment already installed. The home-built apparatus for studying strongly correlated systems with Cs atoms is under construction. A good cooperation with a recognized cold-atoms group from Austria was established with a recently published joint paper in *Physical Review A*.

III. Research programme "Experimental Biophysics of Complex Systems"

Within the program "Experimental Biophysics of Complex Systems" we explore processes and structures of various complex systems (from model systems to the structures in living cells, tissues and even small animals) including the effects of various bioactive molecules like toxins, drugs, etc., as well as of various materials like nanomaterials and medical materials on these systems. Our research is focused on the investigation of the structural properties of different membrane structures such as membrane domains, membrane proteins and glycosaccharide matrix as well as their interactions with various materials that enter into their native environment. Novel spectroscopic and micro-spectroscopic techniques contribute to the understanding of the organization of these supramolecular systems, complex cell and tissue responses as well as opening up new possibilities to design new medical materials, like scaffolds for tissue regeneration as one of the most relevant problems in the current aging population of developed countries. In addition, we focus on medical method optimization, like tumour treatment methods, magnetic resonance imaging and the mathematical modelling of thrombolysis, magnetic resonance microscopy in forestry, wood science and food processing as well as to restricted diffusion research.

One of the hottest topics in biophysics is the study of the interactions between novel materials and cells, especially from the bioactivity and bio-compatibility points of view, which we explore by applying novel micro-spectroscopies. We upgraded our system for fluorescence microspectroscopy, which enables us to acquire fluorescence spectra from small volume elements of the sample and thus to detect physical changes in the local molecular environment of fluorescent probes, with new acquisition and analysis routines. By changing imaging sequence, introducing a spectral model, and implementing efficient computer simulations, we improved the spectral resolution and bleaching correction reliability. These advances - combined with custom designed environmentally sensitive probes enabled us to observe phase transitions of single liposomes (Figure 23), to detect membrane microdomains, i.e., molecular motional patterns, and to determine the local pH in different parts of the cell. With the new system we can now use photobleaching of the probes to obtain new molecular information, which we showed when studying the influence of the B₂ vitamin on cell-membrane resistance to external amphiphilic molecules. As a part of our cell-nanomaterial interaction research, we were investigating the rates and mechanisms of cells' uptake of titanate nanoparticles. The system for micromanipulation was used for research on the dynamics and strength of cell attachment to macrostructured biomedical materials which are used as models for potential artificial tissue scaffolds.

In the area of the **design and synthesis of probes** (nitroxide, fluorophore and combination of both in the same molecule) in 2012 the focus was

on the synthesis of fluorescent probes of the rhodamine type. Their fluorescence spectra are sensitive to changes of pH in the local environment. We have synthesized derivatives of rhodamine labelled mannose, showing high affinity for binding to DC-SIGN receptor on dendritic cells. Binding to the DC-SIGN receptor triggers the process of endocytosis. In this way we have prepared useful molecular tools for the study of cellular structures (e.g., lys-

osomes) and transport mechanisms (e.g., the proposed internalization of the HIV virus), which can be studied by fluorescence micro-spectroscopy. We continued with the development of fluorescent probes of the coumarin type that are sensitive to the local environment (polarity).

The interaction of cancerostatic perifosine (OPP) with different cell lines was investigated by EPR, using a home-developed computer program EPRSIM. Perifosine belongs to the group of alkylphospholipids, a new class of anticancer agents, targeting directly the cell membrane and not DNA and showing a selective apoptotic response in tumour cells, sparing normal cells. The influence of OPP on the membrane fluidity of OPP-resistant MCF7, and OPP-sensitive MT3 breast-cancer cell lines, as well as the accumulation of spin labelled OPP in cells was investigated. The results were compared to those obtained on mouse fibroblast (L929) cell lines. OPP increases the membrane fluidity of all cell lines. However, irrespective of the finding that spin-labelled OPP accumulates better in the sensitive MT3 cells as in the less sensitive MCF7 cells, the changes in membrane fluidity are less pronounced in MT3. Our results show no correlation between the cell membrane fluidity, its changes under the influence of OPP and the sensitivity of cells to OPP. The only correlation we found was between OPP sensitivity and the cell growth rate.

In collaboration with the Biotechnical Faculty of Ljubljana the properties of a new class of liposomes prepared from archeal lipids (archeosomes) was investigated by EPR and fluorescence spectroscopy. It was found that the pH of the growth medium in the range between pH6 and pH8 does not influence the fluidity of the archeosome membrane. By computer simulation of EPR spectra we have found that the membranes are heterogeneous, but become homogeneous at temperatures above 70°C.



Figure 20. Wear of pure iPP and nanocomposites of iPP and MoS, nanotubes.

In the article "Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli" published in Thrombosis Research, we showed that the shape of platelet inclusions in the blood clot can also be influenced by the flow of blood in the area of the clot formation and not only by the biochemistry of the corresponding processes.

In collaboration with the Veterinary Faculty of Ljubljana we introduced the EPR method with spin trap Fe(DETC), to measure the production of a reactive nitric oxide radical (NO) in organs of live animals. We detected the formation of NO in organs of mice after a single oral gavage with live *Escherichia coli*. The measurements indicate an early systemic inflammatory response to the infection. Our investigations so far show EPR as a reliable and efficient method for the detection of NO radicals in living organisms.

One of our main activities is also the study of membrane structuring (Figure 24). In this respect it is important to note that different time and distance scales of methods can lead to very different conclusions regarding the stability of the heterogeneous structure of membranes. We are therefore trying to study observed phenomena and processes with complementary methods. This enables us to better understand the complex problems that we encounter. For example, beside the EPR method we have studied the interaction of cancerostatic OPP with lipid membranes also by attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR). Consequently, we were able to confirm the influence of the composition of membranes on the level of OPP interaction with membranes. We were also able to exclude the influence of spin probes used in EPR on the OPP action, while no molecular probes are required for ATR-FTIR. The second example is the application of ATR-FTIR to examine the influence of protonation on the dynamics of the transformation of molecular bonds during the transition of a fluorescent dye from a cyclic to an open structure.

With the help of molecular dynamics (MD), we calculated the difference in the rotational diffusion of spin labels attached to the peptide, and surrounded by water or membrane. These results are the key to improving the empirical approximations of side-chain conformational space modelling (CSM). Such estimates allow us to significantly reduce the computational time needed for determining the size of the side-chain conformational space. This also enables us to solve inverse problems - for example, the structural characterization of membrane proteins. We found that the diffusion of the spin label in the membrane is approximately 5 to 10 times slower, but surprisingly the size of the available conformational space is very similar to the size available in water. We also used MD to select the 17 most appropriate cysteine mutants of a mechanism as a function of gate polarity. very interesting peptide, the N-terminal part of β -defensin, with has a different 3D structure in



Figure 21. The drain current as a function of the gate voltage at different values of the gate voltage VGS indicates $\sim 10^5 x$ on/off ratio. The scheme presents an electron and hole conduction

a membrane or water environment. Peptide synthesis is still relatively expensive; by using MD simulations we can estimate the **minimum number of key mutants** needed for structural characterization. The resulting structure



Figure 22. Atomic resolution STM image of Sb(111), showing a subsurface defect with 3-fold symmetry. (size $12 \times 12 \text{ nm}^2$, $I_1=76 \text{ mV}$, $U_1=0.8 \text{ nA}$, T=5K)

will be compared to the results of NMR and will highlight the benefits of our (CSM) method for the structural characterization of membrane proteins.

We confirmed that the coating of **titanate nanomaterials** on polyethylene terephthalate (PET) exhibits antimicrobial activity, even when exposed to ordinary fluorescent lamps. In comparison with conventional disinfection processes, such as chemical and steam cleaning, maintaining clean surfaces with the antimicrobial coatings is potentially much less demanding and does not leave behind harmful chemical residues. Given the encouraging results of the antimicrobial activity of titanate nanocoatings, we started to develop a prototype of air and waste-water cleaners.

We have shown that **dimerization of factor Xa** plays an important role in the process of blood clotting or coagulation, in collaboration with researchers from the University of North Carolina. Our results demonstrate that the dimerization site and factor Va-binding site are both located in the catalytic domain of factor Xa and that these sites are linked thermodynamically. We assume that the linkage between the dimer interface and factor Va-binding regions of factor Xa may have a physiological significance in blood coagulation. We speculate that factor Xa dimerization is a mechanism that limits prothrombinase formation when blood clotting is undesirable. We are investigating this possibility using model membranes.

Thrombolysis is a process in which the addition of specific reagents to the bloodstream can dissolve blood clots. So far, thrombolysis was in the literature dealt primarily as a biochemical process. However, in the last few

years we have shown that mechanical forces on the flow of the blood clot are also very important for successful thrombolysis. Therefore, thrombolysis can also be regarded as a kind of corrosion-erosion process. In the past year we published two articles which present a model of thrombolysis as a corrosion-erosion process: "Analysis of blood clot degradation fragment sizes in relation to plasma flow velocity".



Figure 23. Comparison of fluorescence microscopy (left column) and micro-spectroscopy (right column; colours code the position of fluorescence spectrum maximum). Upon phase transition of DPPC liposomes, the spectrum of fluorescent probe SPP268 shifts for approx. 1.5 nm.

Magnetic resonance imaging is a useful tool to show the **heterogeneity of blood clots**. With this method we can distinguish between areas that are predominantly composed of platelets, and are resistive to thrombolysis and areas that are predominantly composed of red blood cells and are more susceptible to thrombolysis. In the published article, we showed that the shape of the platelet inclusions in the blood clot can be explained by the flow of blood in the area of clot formation: "Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli. *Thromb. res.*., 2012, vol. 129, issue 2, str. 158-163."

Magnetic resonance imaging (MRI) was used to study **water distribution and its mobility** in the common bean during soaking at room temperature and cooking of pre-soaked and dry bean. To obtain the total water uptake, a combination of two MRI methods were used: a 3D RARE method that emphasizes the area where highly mobile (bulk) water is present and the signal of low mobile (bound) water is weak or even not observed and a 3D SPI method that emphasizes the area where water restricted in motion is present, but suppressing the bulk water signal owing to the short repetition time. It was shown that by the combination of the 3D SPI and the 3D RARE imaging techniques a complete insight into water distribution in the bean can be obtained and simultaneously tracing of mobile and bound water that penetrated into the bean seed is feasible.

Controlled drug-delivery systems are widely used in the pharmaceutical industry because of their numerous advantages. For hydrophilic polymers, it is generally accepted that, once in contact with body fluids, they hydrate and swell, forming a gel layer that regulates the penetration of body fluids into the tablet and the dissolution of the incorporated drug. Therefore, the knowledge of the gel layer characteristics is of crucial importance for the

use of controlled drug delivery systems. A combination of different MRI methods enables an accurate determination of the medium penetration into the tablet as well as hydrogel formation *in situ*. This approach has been used to determine the influence of the highly soluble incorporated drug in matrix tablets of xanthan on the kinetics of medium penetration and hydrogel formation. The influence of the drug was studied in media with different pH and ionic strengths. The impact of the drug on the hydrogel thickness was found to be dependent on the medium conditions. The drug does not change the hydrogel thickness in a water medium, whereas in acid medium the presence of the drug results in thinner hydrogel. The increased ionic strength in water medium also leads to the formation of the thinner hydrogel layer, while the effect of NaCl in HCl pH 1.2 medium being very small.

Magnetic resonance imaging allows **monitoring of the distribution of electric current density** in the conductive samples. By using current images in several different arrangements of electrodes, it is possible to determine the electrical conductivity of the sample and consequently also the electric field for a given electrode arrangement. This is of paramount importance in **electroporation**, which is a method in which by the use of high voltage the cell membrane is a tissue that is made temporarily permeable and therefore absorbs more drugs than normally, as for example anti-cancer drugs.

Magnetic resonance imaging is also very efficient in showing soft tissues in teeth, especially **dental pulp** (Figure 25). This method can be used to study anatomy or dental pulp or may even be used to detect early effects of dental caries on the pulp. Latter can be detected by ADC mapping of the pulp region.

Our research has been supported by a number of international projects financed by the European Union within the Sixth and Seventh Frameworks. It was also supported within the bilateral Slovenian – USA, Slovenian – German and Slovenian – Greek and other scientific cooperations. In 2012, we had cooperations with 108 partners from Slovenia and abroad. Among them

- The high magnetic field centres in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field cente at the University Florida, Tallahassee, Florida, USA
- The ETH, Zürich, Switzerland
- The Ioffe Institute in St. Petersburg, Russia
- The University of Duisburg, the University of Mainz and the University of Saarbrucken in Germany
- The University of California, the University of Utah and the Liquid Crystal Institute, Kent, Ohio, USA
- National Institute for Research in Inorganic Materials, Tsukuba, Japan
- NCSR Demokritos, Greece
- Institut f
 ür Biophysik und Nanosystemforschung OAW, Graz, Austria
- Bioénergétique et Ingénierie des Protéines, CNRS Marseille, France
- Architecture et Fonction des Macromolécules Biologiques, CNRS Marseille, France
- The Max Delbruck Center for Molecular medicine in Berlin
- The Dartmouth Medical School, Hanover, NH, USA
- The Mayo Clinic, Rochester, USA made the above studies possible.

Some outstanding publications in 2012

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- Dolinšek, J.: Electrical and thermal transport properties of icosahedral and decagonal quasicrystals. Chem. Soc. Rev. 41, 2012, pp. 6730–6744
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- 4. Novak, N., Pirc, R., Wencka, M., Kunnjak, Z.: High-resolution calorimetric study of PbMg _{1/3}Nb_{2/3}O₃ single crystal. Phys. Rev. Lett. 109, 2012, 037601-1-5
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Figure 24. Spin label in three different environments: vacuum, water and membrane as calculated in MD.



Figure 25. MRI image of a dental pulp in different stages of caries (lowest - ICDAS 0 to the maximum - ICDAS 6). Images on the left are T_{i} weighted and show the anatomy of the dental pulp, images on the right are corresponding ADC maps in which regions affected by caries appear purple, while healthy pulp is in pink.

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- 1. Zorko, A., Jeglič, P., Potočnik, A., Arčon, D., Balčytis, A., Jagličić, Z., Liu, X., Tchougreeff, A. L., Dronskowski, A. L.: Unconventional magnetism in a nitrogen-containing analog of cupric oxide. Phys. Rev. Lett. 107, 2011, 047208
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- 8. Fukuda, J., Žumer, S.: Ring defects in a strong confined chiral liquid crystal. Phys. Rev. Lett. 106, 2011, 097801
- 9. Čopar, S., Žumer, S.: Nematic braids: topological invariants and rewiring of disclinations. Phys. Rev. Lett. 106, 2011, 177801
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- 11. Tkalec, U., Ravnik, M., Čopar, S., Žumer, S., Muševič, I.: Reconfigurable knots and links in chiral nematic colloids. Science (Wash. D.C.) 333, 2011, p. 62
- 12. Osterman, N., Vilfan, A.: Finding the ciliary beating pattern with optimal efficiency. Proc. Natl. Acad. Sci. U. S. A. 108, 2011, 15727
- 13. Muševič, I., Žumer, S.: Liquid crystals : maximizing memory. Nature Materials 10, 2011, p. 266

Awards and appointments

- 1. Primož Koželj: Prešern award of the Faculty of mathematics and Physics for Diploma thesis, University of Ljubljana, Ljubljana, Electrical, magnetic, and thermal properties of the δ-FeZn10 complex intermetallic phase,
- 2. Samo Kralj: Golden sign, Maribor, University of Maribor
- 3. Miha Škarabot, Igor Muševič: Luckhurst Samulski Prize, Mainz, Liquid Crystals
- 4. Nikola Novak: Best paper award, Ljubljana, 4th Student Conference of the Jožef Stefan International Postgraduate School, Jožef Stefan International Postgraduate School
- 5. Gregor Posnjak: Prešern award of the Faculty of mathematics and Physics for Diploma thesis, Ljubljana, University of Ljubljana, Magnetic structure determination of one-dimensional antiferromagnet CuSe2O5 with neutron scattering
- 6. Brigita Rožič: Slovenian National L'oreal-UNESCO fellowship "For Women in Science 2012", Ljubljana, L'Oreal Slovenia d. o. o., Slovenian National commision for UNESCO and Slovenian Science Foundation
- 7. Uroš Tkalec: Glenn H. Brown Prize, Mainz, International Liquid Crystal Society

Organization of conferences, congresses and meetings

- 1. Workshop on Assembling of Superstructures in Soft matter, Ljubljana, Slovenia, 11.–13. 10. 2012
- 2. 8th Physicists Conference in Basic Research, Rimske Toplice, Slovenia, 19. 10. 2012

Patent granted

 Igor Muševič, Matjaž Humar, Spherical liquid crystal laser, SI23567 (A), Urad RS za intelektualno lastnino, 31.5.2012

INTERNATIONAL PROJECTS

- NMR Spectrometer 1. Korea Basic Science Institute Prof. Janez Dolinšek 2. MERCK - AFM investigations Merck KGaA Asst. Prof. Miha Škarabot 7. FP - HIERARCHY: Hierarchical assembly in controllable matrices; 215851, PITN-3. GA-2008-215851 European Commission Prof. Igor Muševič 7. FP - UNCOSS: Underwater coastal sea surveyor 4. European Commission Prof. Robert Blinc 7. FP - DIAGNO-RAIL: Combining innovative portable visual, accoustic, magnetic and 5. NMR Methods with In-situ chemical diagnostic tools for effective failure assessment and maintenance strategy of rail and subway systems European Commission Prof. Janez Dolinšek FP - LEMSUPER: Light element molecular superconductivity: An interdisciplinary 6. approach European Commission Prof. Denis Arčon FP - ESNSTM: Electron spin noise scanning tunneling microscopy 7. European Commission Prof. Janez Dolinšek FP - NanoMag: Magnetic nanoparticles and thin films for spintronic applications and high performance permanent magnets European Commission Prof. Janez Dolinšek Structure and mechanism of cytoplasmic dynein HFSP - International Human Frontier Asst. Prof. Andrej Vilfan 10. COST MP1003: ESNAM - European scientific network for artificial muscles COST Office Prof. Boštjan Zalar 11. COST; IMC-SRM: Network for intermetallic compounds as catalysts for steam reforming of methanol COST Office Prof. Janez Dolinšek 12. NATO ARW 984375: Magnetic resonance detection of explosives and illicit materials, 2.-7. 9. 2012, Turkey NATO Asst. Prof. Tomaž Apih 13. COST MP1201: Rational design of hybrid organic-inorganic interfaces: The next step towards advanced functional materials COST Office Dr. Polona Umek
 - Hierarchy Workshop 2012: Workshop on assembling of superstructures in soft matter Prof. Igor Muševič
 - 15. Dielectric and electocaloric properties of advanced relaxor dielectric polymer films and nanotubes
 - Slovenian Research Agency Asst. Prof. Vid Bobnar
 - 16. Geometrically frustrated quantum magnetism
 - Slovenian Research Agency Dr. Andrej Zorko
 - 17. BI-FR/11-12-PROTEUS-008: Novel states of matter induced by frustration in quantum magnets
 - Slovenian Research Agency
 - Dr. Andrej Zorko 18. Hydrogen storage in metal hydrides and nanomaterials Slovenian Research Agency
 - Asst. Prof. Tomaž Apih
 - Factor Xa dimerization and its role in prothrombinase complex formation and activity on membrane surfaces Slovenian Research Agency
 - Dr. Marjeta Šentjurc
 - 20. Syntesis, microscopy characterization and magneto resonance study of new functional nanomaterials Slovenian Research Agency
 - Dr. Polona Umek
 - BI-FR/12-13-PROTEUS-001: Unconventional ground states of quantum matter Slovenian Research Agency Dr. Martin Klanišek
 - Exotic electronic properties arising from geometrical symmetry Slovenian Research Agency Prof. Denis Arčon

RESEARCH PROGRAMS

- 1. Magnetic resonance and dielectric spectroscopy of "smart" new materials Prof. Janez Dolinšek
- 2. Physics of soft matter, surfaces and nanostructures Prof. Slobodan Žumer
- Experimental biophysics of complex systems Prof. Janez Stepišnik

R & D GRANTS AND CONTRACTS

- 1. Dentin evolution detected by spectroscopic means
- Prof. Janez ŠtrancarNovel ground states and quantum critical points in low-dimensional quantum spin systems
- Dr. Andrej Zorko 3. Use of nanoparticles as additives in lubricants and in tribology
- Prof. Maja Remškar
- Optical microresonators based on liquid crystals Prof. Igor Muševič
- New metallic materials for thermal storage of digital information Prof. Ianez Dolinšek
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- Theory of the nematic nanodroplet and ordering of DNA, encapsidated in simple viruses
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- Nanomaterials and Scaffolds preparation and characterization Prof Janez Štrancar
- 27. CONPHIRMER:Counterfeit pharmaceuticals interception using radiofrequency methods in realtime

Asst. Prof. Tomaž Apih

NEW CONTRACTS

 A spectrometer for automatic 14N nuclear quadrupole resonance characterization of new substances

Gorenje Household Appliances, d. d. Dr. Alan Gregorovič CONPHIRMER: Counterfeit pharmac

 CONPHIRMER:Counterfeit pharmaceuticals interception using radiofreqency methods in realtime

VISITORS FROM ABROAD

- 1. Dr. Helena Godinho, Instituto Superior de Tehnico, Lisbon, Portugal, 15.-21. 1. 2012
- Dr. Pedro Sebastiao, Instituto Superior de Tehnico, Lisbon, Portugal, 15.–21. 1. 2012
 Dr. Igor Gvozdovskyy, Institute of Physics, National Academy of Sciences of Ukraine, Nati
- Kyiv, Ukraine, 23. 1.-17. 2. 2012
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- 11. Dr. Uliana Ognysta, Institute of Physics, National Academy of Science of Ukraine, Kyiv, Ukraine, 1. 3.–10. 4. 2012, 27. 5.–15. 7. 2012, 30. 9.–31. 10. 2012
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- 14. Dr. Mutsuo Igarashi, Department of Applied Physics, Gunma National college of Technology, Maebashi, Japan, 10. 3.–15. 3. 2012
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- 18. Dr. Nikolaus Nestle, BASF, Heidelberg, Germany, 24.-27. 4. 2012
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- 20. Dr. Jin Bae Lee, Korea Basic Science Institute, Daejeon, South Korea, 14. 5.-21. 5. 2012
- 21. Dr. Won G. Hong, Korea Basic Science Institute, Daejeon, South Korea, 14. 5.-21. 5. 2012
- 22. Songi Han, Korea Basic Science Institute, Daejeon, South Korea, 14. 5.-21. 5. 2012
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- Prof. Stephan Herminghaus, Max Planck Institute, University of Gottingen, Gottingen, Germany, 5.-8. 6. 2012
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- 27. Dr. Silviu Preda, Ilie Murguescu Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania, 16.-27. 7. 2012
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- 32. Prof. Jin Keun Seo, Yonsei University, Seoul, South Korea, 13.-16. 11. 2012
- 33. Prof. Oh In Kwon, Kunkuk University, Seoul, South Korea, 13.-16. 11. 2012
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58. Andraž Krajnc, B. Sc., left 01.12.12

36. Dr. Andreja Jelen, left 01.10.12

64.

- 66. Dr. Adam Ostrowski
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- 74. Iztok Urbančič, B. Sc.
- 75. Bojana Višić, B. Sc.
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- 78. Venkata Subba Rao Jampani, M. Sc.
- 79. Sandra Kure, B. Sc., left 18.06.12
- 80. Ivan Kvasić, B. Sc.
- 81. Bojan Ložar, B. Sc., died 16.01.12
- 82. Alma Mehle, B. Sc.
- 83. Maryam Nikkhou, M. Sc.
- 84. Milan Rožmarin, B. Sc.

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ORIGINAL SCIENTIFIC ARTICLE

- 1. Gerardo Abbandonato, Donata Catalano, Valentina Domenici, Boštjan Zalar, "²H NMR orientational study of a probe dissolved in nematic solution and, used as crosslinker, in a liquid crystalline elastomer", *Liq. cryst.*, vol. 39, no. 2, pp. 165-174, 2012.
- Tetsuo Asaji, Joshiharu Ito, Janez Seliger, Veselko Žagar, Anton Gradišek, Tomaž Apih, "Phase transition and ring-Puckering motion in a metal organic perovskite [(CH₂)₃NH₂][Zn(HCOO)₃]", *J. phys. chem., A Mol. spectrosc. kinet. environ. gen. theory*, vol. 116, no. 51, pp. 12422-12428, 2012.
- 3. Franci Bajd, Matej Kranjc, Damijan Miklavčič, Igor Serša, "Current density imaging during tissue electroporation", *Pril. Maked. akad. nauk. umet., Odd. biol. med. nauki*, vol. 33, no. 1, pp. 367-372.
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- 6. Franci Bajd, Jernej Vidmar, Andrej Fabjan, Aleš Blinc, Eduard Kralj, Nina Bizjak, Igor Serša, "Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli", *Thromb. res.*, vol. 129, issue 2, pp. 158-163, 2012.
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- 10. Tomaž Požrl, : doctoral dissertation, Ljubljana, 2012 (mentor Jurij F. Tasič).
- 11. Robert Repnik, : doctoral dissertation, Maribor, 2012 (mentor Ivan Gerlič; co-mentor Samo Kralj).
- 12. Brigita Rožič, *Giant energy-conversion effects in soft and solid advanced materials:* doctoral dissertation, Ljubljana, 2012 (mentor Zdravko Kutnjak).
- 13. Mitja Rupreht, : doctoral dissertation, Maribor, 2012 (mentor Vladimir Jevtič; co-mentor Igor Serša).
- Uroš Rozina, Adaptive filtering of VEP and ERG signals in LabView: master's thesis, Ljubljana, 2012 (mentor Marko Topič; co-mentor Dušan Ponikvar).
- 15. Polonca Stopar, *Evaluation of pH dependent rhodamine type fluorescent compounds:* master's thesis, Ljubljana, 2012 (mentor Janez Mravljak; co-mentor Stane Pajk).

DEPARTMENT FOR COMPLEX MATTER

F-7

The research within the Department for Complex Matter encompasses a variety of research fields, ranging from the synthesis of new materials to fundamental investigations of elementary excitations in complex systems. These include anything from nano-biosystems and biomolecules to superconductors and nanowires. The experimental methods used are suitably diverse, from synthetic chemistry to biomedicine and femtosecond laser spectroscopy and magnetometry. Last year's research achievements are thus quite diverse, but we are able to report on breakthroughs in a number of areas.

The activities in the department can be grouped into a number of thematically inter-related research areas. Nanomaterials science research is focused on investigations into the fundamental properties and applications of MoSI molecular wires, crossing into the physics and nanoscience of macromolecular biological systems such as DNA and cilia, and venturing into quantum molecular electronics and nanoelectronics. These and other materials, such as strongly correlated systems, electronically ordered systems and superconductors were investigated using advanced femtosecond spectroscopy techniques. In many areas we have introduced new materials, technologies and techniques.

The year 2012 was very special for the department, in that a large effort was expended on setting up new midand long-term research areas for future. In particular, new techniques were being developed for the study of non-

equilibrium phase transitions, involving both theoretical and experimental work. As a result of these efforts, the department's head was awarded an ERC advanced grant for the study of "Trajectories of complex systems through symmetry breaking phase transitions" which utilizes these new techniques and methods.

In parallel, a significant amount of work was devoted to planning and setting up new equipment and the development of new technologies for

nanoscience and nanoelectronics, which was made available through the Centre of Excellence in Nanoscience and Nanotechnology – Nanocenter. The department thus acquired a new AFM/Micro-Raman system with low-temperature vacuum capability, and a significant share in a FIB dual-beam microscope, both of which are currently fully operational. In addition, a new low-temperature four-probe STM/AFM system was developed with Omicron, which is a unique instrument enabling unprecedented 4-contact measurements of surface transport on the nanoscale. The instrument is to be installed in the latter half of 2013.

Ultrafast studies of electron dynamics in correlated systems

The field of research of relaxation processes of photo-excited electrons in correlated electron systems remains one of our main research topics. Several experimental studies of carrier relaxation phenomena in correlated electron systems with various degrees of correlation have been performed using femtosecond time-resolved techniques.

The aim of the ongoing research is to gain additional information about the nature of the low-lying excitations in these materials, and to explore the nature and strength of the interactions of electrons with other low-lying excitations. Femtosecond spectroscopy has been instrumental in elucidating the nature of the electronic excitations in superconductors, since it allows us to distinguish different components by their lifetimes. Moreover, the relaxation kinetics can yield valuable information about the mechanism for superconductivity.

The relaxation of the non-equilibrium electron distribution created by femtosecond excitation can be viewed as a combination of two processes: thermalization, where the electrons exchange energy with each other to approach an equilibrium distribution, and electron energy relaxation, where the electrons give their excess energy to other excitations, such as phonons. To date, the analysis of femtosecond relaxation measurements has been based on the assumption that thermalization is much faster than energy relaxation. The calculated transient electron distribution, the linear increase of the relaxation time with temperature and the intensity independent relaxation behavior all suggest that in high-temperature superconductors as well as in

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We have studied the electron relaxation dynamics of 14 samples from the pnictide, cuprate, and bismuthate compound families, using femtosecond optical pump-probe spectroscopy. We show that T_c depends systematically on the primary electron-energy relaxation rate $1/\tau_1$.





conventional metals this assumption is generally not fulfilled. We propose a more accurate description, which yields more reliable values for the strength of the electron-phonon interaction determined from the measured relaxation rates. This work is published in **Journal of Applied Physics**, **112605** (2012).

The origin of high critical temperature (T_c) superconductivity is still remarkably elusive. To gain an insight into the high- T_c mechanism we need experiments that identify the parameters that determine T_c and link them to the interaction(s) that establish the superconducting state. We show that T_c depends systematically on the primary electron energy relaxation rate $1/\tau_1$. We have studied the electron relaxation dynamics of 14 samples from the pnictide, cuprate, and bismuthate compound families, using femtosecond optical pump-probe spectroscopy. The non-monotonic T_c ($1/\tau_1$) has one characteristic maximum at intermediate relaxation rates (~16 ps⁻¹ at room temperature). We found that $1/\tau_1$ correlates with the length of the crystallographic *a*-axis, which is a measure of the strain in the Cu-O (Fe-As, Bi-O) planes. We propose to assign $1/\tau_1$ to the electron-phonon interaction and briefly discuss the implications on the possible superconducting mechanism. This work has been submitted for publication. A preprint can be found at **arXiv:1205.4978**.

We continued our research on the relaxation of quasiparticles in pnictide superconductors. We systematically investigate the photoexcited (PE) quasi-particle (QP) relaxation and low-energy electronic structure in electron-doped Ba(Fe_{1-x}Co_x)₂As₂ single crystals as a function of Co doping. In the orthorhombic spin-density-wave (SDW) state a bottleneck associated with a partial charge-gap opening is detected. In the superconducting (SC) state an additional relaxational component appears due to a partial (or complete) destruction of the SC state proceeding on a sub-0.5-picosecond timescale. From the SC component saturation behavior the optical SC-state destruction energy is determined near the optimal doping. The *T*-dependence of the transient reflectivity amplitude in the normal state

We clearly identified intrinsic topological defect annihilation processes in TbTe_{3} on a timescale of ${\sim}30~\text{ps.}$

is consistent with the presence of a pseudogap in the QP density of states. The polarization anisotropy of the transients suggests that the pseudogap-like behavior might be associated with a broken point symmetry resulting from nematic electronic fluctuations persisting up to ~ 200 K at any *x*. The second moment of the Eliashberg function, obtained from the relaxation rate in the indicates a moderate electron phonen coupling ~ 0.3 that decreases with

metallic state at higher temperatures, indicates a moderate electron phonon coupling, ~0.3, that decreases with increasing doping. The results were published in Phys. Rev. B 86, 024519 (2012).

We also investigated the temperature and magnetic field dependent photo-excited electron and spin relaxation in $\text{EuFe}_2(\text{As}_{0,7}\text{P}_{0,3})_2$ (EFAP) pnictide superconductor and parent non-superconducting EuFe_2As_2 (EFA) by means of optical pump-probe femtosecond spectroscopy. A remarkable change of the quasiparticle relaxation dynamics at the antiferromagnetic (AFM) SDW transition temperature of 200 K is observed in EFA, consistent with a bottleneck formation due to a charge gap opening.

In both samples we observe at low temperature the emergence of a slow anisotropic photo-induced relaxation component concurrent with Eu²⁺ spin ordering. The magnetic field dependence of the relaxation in the superconducting EFAP is different than in the non-superconducting EFA. In EFA we observe switching of the optical-transients anisotropy with increasing magnetic field attributed to a field-induced antiferromagnetic (AFM) to ferromagnetic (FM) phase transition. In the superconducting EFAP a large coherent magnon oscillation is observed at a similar metamagnetic transition. The oscillation is absent in the transient magneto-optical Kerr effect, suggesting an interplay between the Eu²⁺ spin and the charge degrees of freedom.

We have shown for the first time complete switching in 1T -TaS₂ between the ground state and a new stable hidden state by a single laser pulse.

A significant effort was invested into an investigation of dynamical phase transitions in superconducting and CDW systems. This work is the beginning of a larger project, so most results are not yet completely ready for publication, while others are in the publication process.

In the cuprate superconductor $La_{1.9}Sr_{0.1}CuO_4$ we investigated the trajectory of the superconducting order parameter Ψ through the normal-to-

superconductor transition under varying ultrafast quench conditions. Using a 3-pulse technique we isolated the trajectory of Ψ from single-particle processes on short timescales. Self-consistent modeling of the system trajectory using time-dependent Ginzburg-Landau theory and vortex creation according to the Kibble-Zurek mechanism describes the experimental data well, significantly advancing our understanding of the behaviour of the normal-to-superconductor transition under highly nonequilibrium conditions. The manuscript is in preparation for submission to Physical Review Letters.

By means of the 3-pulse time-resolved optical spectroscopy technique we also investigated underdoped $Bi_2Sr_2CaCu_2O_{8*d}$. Two regimes in the power of the destruction (D) pulse reveal different phenomena: (i) For weak D pulses the PG is unimpaired but the superconducting (SC) state is partially destroyed. Below the critical temperature the behaviour is qualitatively similar to $La_{1.9}Sr_{0.1}CuO_4$ with a somewhat faster SC state destruction and recovery times. The characteristic footprint of the SC response was also detected at temperatures above T_c , indicating the presence of the superconducting fluctuations up to 20 K above the critical temperature. (ii) For strong D pulses the

pseudogap state (PG) is also destroyed. The PG recovery time shows fluence dependence, suggesting that the origin of the PG is not a single particle effect.

In CDW systems we studied the incoherent recombination of topological defects created during the rapid quench of a charge-density-wave system through the electronic ordering transition. Using the above-mentioned 3-pulse femtosecond optical spectroscopy technique we follow the evolution of the order parameter over a wide range of timescales after the quench. By careful consideration of thermal processes we clearly identified intrinsic topological defect annihilation processes in TbTe₃ on a timescale of \sim 30 ps and found a signature of extrinsic defect-dominated relaxation dynamics occurring on longer timescales. A similar effect was also observed in blue bronze and 2*H*-TaSe₂. A manuscript describing this work (arXiv:1208.1105) is currently under consideration for publication in Physical Review Letters.





Figure 1: The photoinduced reflectivity ($\Delta R/R$) transients as a function of temperature at different dopings and probe polarizations in Ba(Fe1-xCox)2As2 (a)-(d), (f)-(j). The vertical lines indicate Tc (full lines), TSDW (dashed lines), and Ts (dotted lines). The phase diagram of Ba(Fe1-xCox)2As2 (e). The investigated-sample dopings are marked by the yellow vertical bars.

so far been very elusive. Commonly, the photo-excited states are transient, and do not show true switching behaviour. We have shown for the first time complete switching in 1T-TaS₂ between the ground state and a new stable hidden state by a single laser pulse. The new photo-excited state or *p*-TaS₂ state is completely stable below T_{oc}~100 K. Switching back reversibly to the ground state is performed using a laser "heat pulse". Remarkably, switching is only observed for pulses shorter than 4 ps, indicating a purely electronic driving mechanism for the transition. The new photo-induced state is characterized by a modified vibrational spectrum, which does not correspond to any known phase or polytype of the material. The change of state is also accompanied by a change of dielectric constant at optical frequencies and DC resistivity, suggesting possible applications for a femtosecond switchable bistable non-volatile memory. The manuscript describing the result is currently in preparation, while a patent application for a bistable memory device based on this principle has already been submitted.

Theoretical studies on the nanoscale

In the hopping magnetoresistance of doped insulators, an applied magnetic field shrinks the electron s-wave function of a donor or an acceptor and this reduces the overlap between the hopping sites resulting in the positive magnetoresistance quadratic in a weak magnetic field. Different from s-states, a weak magnetic field expands the electron wave functions with positive magnetic quantum numbers, and shrinks the states with negative magnetoresistance, which is linear in the field when the orbital degeneracy is lifted. The theory provides a possible explanation of a large low-field magnetoresistance in disordered organic materials. (Physical Review Letters, 108, 186601 (2012)).

The current-voltage characteristics of long and narrow superconducting channels shunted with normal resistors are investigated using the time-dependent Ginzburg-Landau equations for the complex order parameter. We have shown that the switching current is not effected by the shunt. On the other hand, the re-trapping current is increasing with the decreasing of the resistivity of the shunt. When the resistance of the shunt is lower than a certain critical value of the shunt resistance, the current-voltage characteristics do not show hysteretic behavior. (submitted to Physical Review B).

Nanomaterials

Inorganic molecular wires – particularly molybdenum halide or chalcogenide cluster polymers – have emerged as a new type of one-dimensional material with remarkable molecular-scale functionality. Their one-dimensional polymer structure gives rise to some very unusual physical properties. Anionic bridges that bind Mo clusters together into one-dimensional chains are extraordinarily strong, yet highly deformable, giving rise to exceptionally high Young's moduli and nonlinear mechanical properties, respectively. The very weak interaction between individual polymer chains within crystalline bundles leads to the observation of an extreme one-dimensional electronic and magnetic character, on the one hand, and also to an easy dispersion in common polar solvents and ultralow shear moduli on the other. The sulfur atoms within the structure facilitate diverse functionalization chemistry to thiol-containing molecules, such as proteins.

Until now, MoSI MWs were synthesized under a high pressure of ~100 bar and temperatures of 1000 °C or above. To develop a process that can be scaled up, we examined the synthesis under growth conditions that can be realized in chemical vapor deposition (CVD): a lower temperature of 850 °C and a total vapor pressure of 1 bar. We demonstrated that MoSI NWs can be synthesized under these conditions. The resulting material depends strongly on the morphology of the Mo starting material, with a combination of nanostructured Mo foil and Mo powder being the most conducive to long and flexible MoSI NWs. These results are reported in **Synthetic Metals 162**, 1677–1680

(2012). Building on these results, we are now exploring the vertical growth of MoSI NWs for chemisensor and different aptamer/antibody biosensor applications.

Poly(ϵ -caprolactone) (PCL) is one of the most commonly used polymers in biomedical applications, mainly because it is biodegradable. We report, for the first time, on the preparation of composites of Mo₆S₃I₆ with PCL via

Noble-metal nanoparticles were directly deposited on $Mo_6Sylz(8.2 \le y+z \le 10)$ wire bundles either in a solution (water) or on a substrate (SiO₂) at room temperature in a single-step reaction without any additional reducing reagents.

melt mixing in a twin screw extruder. Extensive microscopic examinations of the composites revealed that the nanowires were well dispersed in the PCL matrix, although bundles of Mo₆S₃I₆ ropes were evident at higher loadings. Secondary electron imaging (SEI) showed that the nanowires had formed an extensive network throughout the PCL matrix, resulting in increased electrical conductivity of PCL, by eight orders of magnitude, and an electrical percolation threshold of 6.5x10⁻³ vol%. This means that the Mo₆S₃I₆ nanowires are credible alternatives to CNTs as functional fillers for polymeric materiation.

als for use in electrostatic discharge, EMI shielding, flexible electronic substrate, and electrode applications. These results are reported in **Polymers for Advanced Technology 23**, 149–160 (2012).

The following work sits on the cusp between nano and correlated materials – since it uses a correlated material but performs nanostructuring on it, with no ultrafast electron dynamics:

We have shown that a (positive or negative) charge can be induced by the application of a positive or negative local bias to the surface of a $La_{1.975}Sr_{0.025}CuO_{4+\delta}$ (LSCO) crystal by a conducting atomic force microscope (AFM) tip. The charged regions are found by Auger electron spectroscopy (AES) to have a different stoichiometry from the

We discovered a straightforward technique to synthesize pure Mo nanowires (NWs) from $Mo_6Sylz (8,2 < y + z \le 10)$ NWs as precursor templates. surrounding material, over a depth of a few nanometers and resolution limited width. The rapid relaxation dynamics of the surface potential is consistent with an ionic diffusion process, but that there is a very long, semipermanent change that is present for both bias polarities and does not relax in months. The absence of patterning in a vacuum shows that the modification is mediated by a water meniscus, which can act as an electrochemical

nanocell reactor. For small voltages, the topography is unchanged, even though substantial O is transferred. This thus presents qualitatively a new effect, where electrochemical doping is achieved within the nanocell volume capillary water. Remarkably, the process is completely reversible. Apart from fundamental implications for the heterostructure device construction, such surface charge manipulation could lead to the AFM nanopatterning of superconducting nanoscale devices and applications in memories. These results are reported in **Journal of Physics D: Applied Physics 45**, 125302-1–125302-5.

We report on a simple procedure that enables the efficient and large-scale production of thin bundles of Mo6SyIz($8.2 \le y+z \le 10$) nanowires and their decoration with noble-metal nanoparticles. These MoSI nanowires are grown directly from the elements by optimising the chemical transport reaction conditions. The obtained nanowires self-assemble into bundles of different sizes and orientation. We successfully isolated bulk quantities



Figure 2: Relaxation time of electrons provides the critical temperature of high-temperature superconductors.

of bundles with diameters of up to 80 nm that were several microns long by using controlled ultra-sonication and centrifugation purification in acetonitrile. The isolated bundles formed a stable dispersion in water without added surfactants. Noble-metal nanoparticles were directly deposited on Mo6SyIz($8.2 \le y+z \le 10$) wire bundles either in a solution (water) or on a substrate (SiO2) at room temperature in a single-step reaction without any additional reducing reagents. We discovered that the nanowires act as a reducing and capping agent and can be readily oxidised. We controlled the density of gold nanoparticles on a nanowire bundle by changing the concentration of the chloro-noble metal complex XNMCl4. (NM= Pd, Pt, Au) (X= H,Na,K) in the water solution. Several different methods, including X-ray diffraction, scanning electron microscopy with wavelength dispersive analysis, and transmission electron microscopy were used for the characterisation of the starting nanowires and the final products.

We discovered a straightforward technique to synthesize pure Mo nanowires (NWs) from Mo6SyIz ($8, 2 \le y + z \le 10$) NWs as precursor templates. The structural transformations occur when Mo6SyIz NWs are annealed in an Ar/H2 mixture leading to the formation of pure Mo NWs with similar structures as initial morphologies. Detailed microscopic characterizations showed that large-diameter (>15 nm) Mo NWs are highly porous, while

small diameters (<7 nm) are made of solid nanocrystalline grains. We found that NWs of diameter 4 nm can carry up to 30μ A current without suffering structural degradation. Moreover, NWs can be elastically deformed

over several cycles without signs of plastic deformation. These results are reported in Nanoscale Research Letters 7, 567 (2012). The method has been filed as a world patent with the application number PCT/SI2012/000041 (publication number WO/2012/177224).

Electron dynamics in biological macromolecules

In 2012 we have made important progress in manufacturing single DNA molecule nanocircuits for an investigation of the electron transport properties of DNA complexes with transition-metal ions, i.e., M-DNA. We have defined an optimal geometry for electrical leads with sub-micron gaps adapted for our electrical measurements on

individual DNA molecules. The circuits were produced by e-beam lithography. The macromolecules of M-DNA differ in structure from the common (canonical) B-DNA only by the incorporated divalent transition-metal cations in the interior of the double helix. They were deposited on the nanocircuits by casting a buffer solution in a direction perpendicular to the electrical micro-leads. An AFM picture in Fig 3 shows the individual M-DNA molecules bridging a sub-micron gap between electrical micro-contacts, as prepared with our method. With this method we can now routinely deposit DNA and M-DNA molecules on prepared nanocircuites and measure not only the I-V characteristics of individual DNA/M-DNA molecules under ambient conditions but also the temperature dependences of their electrical conductivity in a broad temperature range (2-300 K). The measurements have shown that the conductivity of a pristine, non-complexed DNA exhibits an activated behavior where the conductivity exponentially decays toward zero as the temperature is lowered from room temperature - a behavior typical for electric insulators. In contrast, the conductivity of an M-DNA molecule has shown a plateau in a middle temperature range (100-200 K) where the conductivity is virtually temperature-independent. Similar behavior were observed recently



Figure 3: An AFM image of long, individual molecules of M-DNA bridging a sub-micron gap between two gold microelectrodes.

in contactless measurements of the microwave cavity loss at 10 GHz on bulk samples (A. Omerzu et al, *Phys. Rev. Lett.* **104**, 156804 (2010)). These results give firm support to the hypothesis that the electron transport in M-DNA is strongly correlated and much more efficient at longer (< 10 nm) distances then in the native DNA.

Soft Matter

In 2012 we continued with investigations of optical holographic patterning in light-sensitive liquid-crystal elastomers (LCEs). These are polymer materials that exhibit a very strong opto-mechanical response, which is why they are promising for applications in various optically manipulated micromechanical devices. We investigated unusual phenomena observed in the vicinity of the phase transition from the nematic to the paranematic phase. The investigations of the kinetics of the holographic recording process were reported in **Materials 5**, 741-753 (2012), while observation of the so-called "hidden holograms" is reported in a paper that is in the publication process in *Phys. Rev. E.* We also investigated the tunability of the grating period of the optical diffraction gratings made from LCEs, which is reported in **Proc. SPIE**, **8556**, 012031-1-4 (2012).

We continued investigations of the effect of inorganic nanotubes and nanowires on the electro-optical properties of nematic liquid crystals and their composites with polymer materials. We performed systematic analyses of the effect of different nanotubes on the switching voltage and switching time of conventional nematic liquid crystals 5CB and E7. After this we extended our work on the use of polymerizable nematic liquid-crystal material RM257 (Merck). The main goal of these efforts is to obtain a polymer-nanotube composite material with an orientationally ordered distribution of nanotubes.

In cooperation with the Faculty of Physics at the University of Vienna we continued with investigations of holographically structured materials that can be used as diffractive elements for the manipulation of cold neutron beams. Different methods for the holographic patterning of composite materials made from photopolymer and

superparamagnetic nanoparticles were analyzed. The main goal of these investigations is the fabrication of a new type of polarizers and analyzers for cold neutrons. The results are reported in: J. Phys., Conference Series 340, 012031-1-4 (2012) and Materials 5, 2788-2815 (2012).

Our investigations of the self-assembling properties of DNA-related molecules were in 2012 focused onto two problems: (i) an analysis of the interaction properties of lipophilic derivatives of all four DNA bases (A, G, C, T) in monomolecular thin films on the water surface (Langmuir films) and (ii) comparative study of the aggregation properties of four very similar G-

Our investigations of the interaction properties of lipophilic derivatives of all four DNA bases (A, G, C, T) in monomolecular thin films on the water surface (Langmuir films) showed that also in thin surface films guanine-derivatives exhibit very different behaviour from the derivatives of other DNA bases. rich DNA oligonucleotides in an aqueous solution. The investigations of the former showed that also in thin surface films guanine-derivatives exhibit very different behaviour from the derivatives of other DNA bases. The results of

A stable nematic suspension can be produced with macroscopic magnetization along the nematic director n. After cooling in magnetic field a monodomain sample is obtained in which the magnetization can be switched by reversing the field.

this work were reported in Colloids & Surfaces B 103, 45-51 (2012). The investigations of the aggregation properties in solution show that all four investigated oligonucleotides self-assemble into G-quadruplex structures. But, in contrast to the expected behaviour, oligonucleotides without the "sticky" GC ends form shorter G4-wire structures than oligonucleotides without the sticky ends. A publication about these results is in preparation.

In cooperation with CO PoliMat we investigated the effect of plasma treatment on water sorption in cellulose fibers. This work is a part of a larger project in medical sciences devoted to the development of new kinds of multifunctional materials for wound

dressing. The results were reported in Mater. Technol. 46, 69-73 (2012). Nematic liquid crystals formed by dimers with an odd flexible spacer exhibit transitions to modulated structures



Figure 4: Brewster angle microscopy (BAM) image of Langmuir film of guanosine derivative with one lipophilic chain. The image was taken during film compression in the two-phase-coexistence region.

and phases with domains of opposite chirality. To test the prediction that the bend elastic constant for odd-membered liquid-crystal dimers can go to zero, causing the transition, we have performed dynamic light-scattering measurements in the two homologues CB7CB and CB9CB. The relaxation rates of the twist and splay modes are only weakly temperature dependent, but that for the bend mode slows down dramatically towards the transition to the modulated phase. At the transition both the bend and twist modes disappear, while the splay relaxation rate increases strongly. The bare splay and twist elastic constants increase slowly with decreasing temperature, while the bend constant decreases by a factor of 1.7 in CB7CB and 2.3 in CB9CB. This result indicates that the modulated phase due to the softening of the bend elastic. The softening of the bend constant is caused by a negative value of third-order invariants in the Landau-deGennes free energy.

We showed that using ferromagnetic platelets, with anchoring at the platelets surface that favours perpendicular orientation of the nematic director at the particles' surface, a stable nematic suspension can be produced with macroscopic magnetization along the nematic director n. Cooling to the nematic phase in the absence of the magnetic field produces a polydomain sample with two opposite states of magnetization parallel to the nematic ordering. After cooling in a magnetic field a monodomain sample is obtained

in which the magnetization can be switched by reversing the field. The existence of this unique ferromagnetic fluid is due to an interplay of nematic elastic interaction that crucially depends on the shape of the particles and magnetic dipolar interaction.

In collaboration with the Department of Condensed Matter Physics (F5) we experimentally studied the behavior of liquid crystals (LCs) under the influence of time-modulated temperature gradients. The absorption of the traveling laser beam in the LC creates a traveling region of elevated temperature. The combination of a temperature-dependent viscosity and the thermal expansion of the liquid results in a fluid flow in the direction opposite to the movement of the hot region. We demonstrated guided flows in the nematic LC and showed that the method enables custom alignment of the LC director on a micrometer scale. The preliminary findings were presented at ILCC 2012.

Nonlinear optics

In the Nonlinear Optics Laboratory we study new materials and their interaction with laser light. Integrated optics is a promising technology; however, better materials will increase its potential. In cooperation with North Carolina State University in Raleigh, USA, we study new concepts of compact light sources on the basis of nonlinear

We have also developed a more compact two-frequency laser source at 9.31 THz. This frequency is sufficiently far away from the water absorption lines and therefore large propagation distances of the THz waves can be realized in devices, e.g., for remote materials testing.

optical conversion of existing lasers into the spectral regions where lasers are not yet available. AlGaN grown by metal-organic chemical vapor deposition (MOCVD) has a great potential for optoelectronic devices emitting and detecting light in the ultraviolet (UV) wavelength regime. We study AlGaN waveguides with an alternating sign of the nonlinear coefficient in regular intervals and allows quasi phase matching.

In cooperation with Rainbow Photonics A.G., a spin-off company of ETH Zurich, we study THz generation with difference frequency mixing.

One way is using a two-frequency optical parametric oscillator to produce pulses with two frequency components of a prescribed frequency difference. We also develop a more compact two-frequency laser source at 9.31 THz. This frequency is sufficiently far away from the water absorption lines and therefore large propagation distances of the THz waves can be realized in devices, e.g., for remote materials testing. The two-frequency laser uses Nd:YAG and Yb:YAG as laser hosts, with emission wavelengths at $1.03 \,\mu\text{m}$ and $1.06 \,\mu\text{m}$.

Biomedical optics

We have investigated the potential of pulsed photo-thermal radiometry (PPTR) for non-contact measurements of laser-induced temperature profiles in strongly scattering biological tissues. Using an original laboratory setup, we

have monitored the laser removal of unwanted tattoos in human volunteers and demonstrated the high value of the obtained information for objective guidance of therapy on an individual patient basis. Using the same technique, we have studied the energy deposition characteristics of a prototype Nd:YAP laser (1342 nm) in the skin of four healthy volunteers, and compared them with those of two customary medical lasers (Nd:YAG and KTP, emitting at 1064 and 532 nm, respectively). The results indicate that the Nd:YAP laser could enable safe and effective non-ablative rejuvenation of sun-damaged skin. Both studies were performed in collaboration with Fotona d.d., Ljubljana.

We have demonstrated that our method provides more accurate and reliable damage-threshold values than earlier proposed approaches. The application of such a protocol could significantly improve the efficacy and safety of several dermatologic laser treatments.

The SFTR profiling technique was also applied for the characterization of laser light absorption in a simple in-vitro model of cutaneous vessel containing a contrast agent based on dedicated polymer nanostructures with ICG dye (collaboration with University of California at Riverside, USA).

Using the same experimental approach, combined with a dedicated numerical model, we have developed a unique method for an objective determination of the maximum safe radiant exposure in the irradiation of human

skin with millisecond laser pulses. We have demonstrated that our method provides more accurate and reliable damage-threshold values than earlier proposed approaches. The application of such a protocol could significantly improve the efficacy and safety of several dermatologic laser treatments, where the radiant exposure is currently selected based on a subjective judgment of the treating physician.

We have participated in a study of selective coagulation of cutaneous vasculature using sequential laser irradiation and millisecond cryogen sprays, performed in an animal model (in collaboration with Beckman Laser Institute at University of California, Irvine, USA).

We have developed a three-dimensional (3D) Monte Carlo (MC) model of light transport in strongly scattering and heterogeneous human skin with rigorous treatment of the analytically defined boundaries between neighbouring tissues. In contrast to the customary implementation of the 3D MC approach, where tissue boundaries are approximated according to the rectangular spatial grid, the results of our model do not depend on the discretization step or minute translations of the spatial grid. The predicted energy deposition in subsurface absorbing structures (e.g., blood vessels) can vary up to 30% between the models, indicating an inherent deficiency of the customary approach.

Biological systems

In collaboration with the *Laboratory for Experimental Soft Matter* at *Faculty of Mathematics and Physics, University of Ljubljana*, we continued the research of biomimetic systems with an emphasis on the analysis of the flow around a single artificial cilium and a study of hydrodynamic coupling among artificial cilia. We used tracer particles to monitor and map the hydrodynamic flow. A comparison with the simple theoretical model revealed

that higher-order terms of the multipole expansion of flow velocity have to be taken into account to match the experimental data. Our findings were published in Beilstein J. Nanotechnol. 2012, 3, 163–171.

Hydrodynamic coupling was studied in a system of artificial cilia, where one cilium was active – actuated with the external field – whereas the other one was passive. We used magneto-optical tweezers to compose the active one from micron-sized superparamagnetic colloidal particles that were subsequently stabilized in chain configuration by the external magnetic field. The passive cilium did not interact with the field therefore its movement directly reflected the motion of the surrounding liquid. A comparison In collaboration with the Laboratory for Experimental Soft Matter at Faculty of Mathematics and Physics, University of Ljubljana, we finished the development of the counter-propagating dual-beam optical tweezers, where two laser beams hold trapped objects with much higher force than in ordinary single-beam tweezers.

of the amplitudes of both cilia gave us exact coupling coefficients and their anisotropy. The results were presented in an invited lecture at a conference in London, while the article is in preparation.

With the same laboratory we finished the development of the counter-propagating dual-beam optical tweezers, where two laser beams hold trapped objects with much higher force than in ordinary single-beam tweezers. The



Figure 5: Bundles of MoSI nanowires decorated with gold nanoparticles.

system will be used to characterize the intermolecular interactions of biologically relevant molecules and to measure the micro-rheological properties of the complex matter.

In collaboration with the Department of Condensed Matter Physics (F5) we developed a theoretical model for the optimization of ciliary beating patterns based on energetic efficiency and used it to search for the most efficient beating pattern of cilia, where the complete stroke is limited to a single plane. Such planar strokes are used by some unicellular organisms, such as Stentor and Opalina. We discovered that the metachronal coordination on a densely ciliated surface of cilia beating in time-symmetric reciprocal manner enables fluid pumping, despite the fact that the Purcell's scallop theorem forbids it on a level of a single cilium. We also showed that some external constraints (for example, limited maximum torque acting on a cilium) can make symplectic waves more efficient than antiplectic ones.

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Organization of conferences, congresses and meetings

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- 2. Adolf Jesih, Andrej Kovič, Aleš Mrzel, Method for a synthesis of quasi-one-dimensional structures of 4d and 5d (Nb, Mo Ta, W) transition metals, SI23768 (A), Urad RS za intelektualno lastnino, 31.12.2012.

INTERNATIONAL PROJECTS

- 1. 7. FP HINTS: Next generation hybrid interfaces for spintronic applications European Commission
- Prof. Viktor Kabanov2. 7. FP COSIT: Compact high brilliance single frenquency terahertz source European Commission
- Prof. Marko Zgonik7. FP ERESIN: Electronic response of single inorganic nanowires European Commission
- Prof. Dragan Dragoljub Mihailović
- COST, Action MP0802: Self-assembled guanosine structures for molecular electronic devices
 - COST Office
- Prof. Martin Čopič
 5. COST, Action MPNS0902: COINAPO Composites of inorganic nanotubes and polymers COST Office
- Prof. Dragan Dragoljub Mihailović
- Organization of the international conference SLONANO 2012, 24.–26. 10. 2012, Ljubljana
- Prof. Dragan Dragoljub Mihailović
- Laser therapy of cutaneous vascular lesions using repetitive irradiation and intermittent cryogen cooling Slovenian Research Agency
- Prof. Boris Majaron
- Age determination of traumatic bruises by combined diffuse reflectance spectroscopy and pulsed photothermal radiometry Slovenian Research Agency Prof. Boris Majaron

- 9. Electron phonon coupling in high-temperature superconductors determined from femtosecond electron relaxation rates Slovenian Research Agency
- Prof. Viktor Kabanov 10. Photonic structures based on polymer-nanoparticle composites Slovenian Research Agency
- Prof. Irena Drevenšek Olenik
 11. Crystal and film growth and time-domain optical spectroscopy investigations of the supeconducting state of the cuprate superconductors
 Slovenian Research Agency
- Asst. Prof. Tomaž Mertelj
- Time resolved optical spectroscopy of collective electronically ordered states in iron based pnictides Slovenian Research Agency
 - Prof. Viktor Kabanov
- Spectrum of the collective excitations of the quasi-one-dimensional conductors with the charge density wave in the equilibrium and nonequilibrium state Slovenian Research Agency Prof. Viktor Kabanov

RESEARCH PROGRAMS

- Light and matter
 Draf Mantin Čaniš
- Prof. Martin Čopič 2. Dynamics of complex nano-systems
- Prof. Dragan Dragoljub Mihailović

R & D GRANTS AND CONTRACTS

- Collective and molecular dynamics of photosensitive liquid crystal elastomers 1 Prof. Martin Čopič
- 2 Molecular elecronics with MoSI nanowires Prof. Dragan Dragoljub Mihailović
- Biomimetic sistems in microfluidic 3 Dr Moica Vilfan
- 4 Molecular motors
- Dr. Natan Osterman

VISITORS FROM ABROAD

- 1. Prof. Eduard Tutis, Institute of Physics, University of Zagreb, Croatia, 10. 4. 2012 Prof. Lise Lyngsnes Randeberg, Department of Electronics and Telecommunications,
- Norwegian University of Science and Technology (NTNU), Trondheim, Norway, 21.-24.5.2012
- Nataša Vujičić, Institute of Physics, University of Zagreb, Croatia, 31. 5. 2012
- Nevena Čelić, Faculty of Science, University of Zagreb, Novi Sad, Serbia, 4. 6. 2012 5. Tetiana Borzda, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, 9.-13. 7. 2012
- Prof. Xinzheng Zhang, TEDA Applied Physics School, Nankai University, China, 6 9.-22.7.2012

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Researchers

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- Prof. Jure Demšar, left 01.08.12 3.
- 4. Prof. Irena Drevenšek Olenik*
- Asst. Prof. Christoph Gadermaier 5.
- Prof. Viktor Kabanov 6.
- Dr. Matjaž Lukač*, left 01.07.12
- Prof. Boris Majaron 8.
- Dr. Marko Marinček*, left 01.07.12 0
- 10. Asst. Prof. Alenka Mertelj 11. Asst. Prof. Tomaž Merteli
- 12. Prof. Dragan Dragoljub Mihailović, Head
- 13. Dr. Aleš Mrzel
- 14. Dr. Aleš Omerzu
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- 16. Dr. Mojca Vilfan

17. Prof. Marko Zgonik* **Postdoctorial associates**

- 18. Dr. Primož Kušar
- 19. Dr. Aleksej Majkić
- 20. Dr. Matija Milanič
- 21. Dr. Natan Osterman
- 22. Dr. Jure Strle

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- Ultrafast electron dynamics in metals and determination of electron-phonon coupling 5. constant in metals and superconductors Prof. Viktor Kabanov
- 6. Cosmology in the lab - femtosecond control of phase transitions in real time Prof. Dragan Dragoljub Mihailović
- 7 Center of competence biomedical engineering: CC BME Prof. Boris Majaron
- Dr. Liqin Tang, TEDA Applied Physics School, Nankai University, China, 9.-22. 7. 2012
- Dr. Yasunori Toda, Department of Applied Physics, Hokkaido University, Sapporo, Japan, 17.-19. 9. 2012
- 9 Dr. Migaku Oda, Department of Applied Physics, Hokkaido University, Sapporo, Japan, 17.-19.9.2012
- 10 Dr. Uwe Bovensiepen, University Duisburg-Essen, Faculty of Physics, Duisburg, Germany, 4.-5. 10. 2012
- Dr. Valentin Alek Dediu, CNR-ISMN Institute, Bologna, Italy, 19.-21. 11. 2012 11 12. Dr. Alberto Riminucci, CNR-ISMN Institute, Bologna, Italy, 10.-11. 12. 2012

Postgraduates

- 23. Vladimir Baranov, B. Sc.
- 24. Miloš Borovšak, B. Sc.
- 25. Jože Buh, B. Sc. Gašper Kokot, B. Sc.
- 26. 27. Andrej Kovič, B. Sc.
- 28. Dr. Andrej Petelin, left 01.07.12
- 29. Anna Pogrebna, B. Sc
- 30. Ljupka Stojčevska, B. Sc.
- 31. Martin Strojnik, B. Sc.
- 32. Peter Topolovšek, B. Sc.

33. Luka Vidovič. B. Sc. **Technical officers**

- 34. Alessandro Lukan, B. Sc., retired 01.06.12
- 35. Damian Svetin, B. Sc.
- 36. Petra Šutar, B. Sc.

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- 37. Martina Knavs, B. Sc.
- 38. Janja Milivojević 39. Nataša Zakrajšek, B. Sc

Note: * part-time JSI member

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(INVITED LECTURE)

1. Matija Milanič, Boris Majaron, "Pulsed photothermal depth profiling of tattoos undergoing laser removal treatment", In: *Photonic therapeutics and diagnostics VIII: 21-24 January 2012, San Francisco, California, United States,* (Proceedings of SPIE, vol. 8207), Nikiforos Kollias, ed., Bellingham, SPIE, 2012, pp. 82070G-1-82070G-12.

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1. Tinka Bačič, Mojca Vilfan, Simona Strgulc-Krajšek, Jasna Dolenc Koce, Vane Krajšek, *Spoznavamo naravo 6: učbenik za naravoslovje v 6. razredu osnovne šole*, 2. dopolnjena in popravljena izd., Preddvor, Narava, 2012.

PATENT APPLICATION

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- 2. Andrej Kovič, Adolf Jesih, Aleš Mrzel, *The procedure for the synthesis of* 4d and 5d (Nb, Mo Ta, W) nitrites of transition metals in the form of quasi-one-dimensional structures, P-20120057, Urad RS za intelektualno lastnino, 22.2.2012.

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PATENT

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MENTORING

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- Aljaž Drnovšek, Optimization of MoSIx selective gas nanosensor: master's thesis, Ljubljana, 2012 (mentor Dragan Mihailović).
- a. Andraž Rešetič, Structure and microrheological properties of binary colloids: master's thesis, Ljubljana, 2012 (mentor Alenka Mertelj).
 4. Peter Topolovšek, Doping and transformations of Mo₆S_{9-x}I_x nanowires
- 4. Peter Topolovšek, Doping and transformations of $Mo_6S_{9-x}I_x$ nanowires with alkali and alkaline earth metals: master's thesis, Ljubljana, 2012 (mentor Dragan Mihailović).

DEPARTMENT OF REACTOR PHYSICS **F-8**

- During the past year we have been working mainly on:
- theoretical, experimental and applied reactor physics
- plasma physics
- neutron-transport calculations
- semiconductor physics
- medical physics

In the field of **reactor physics** we continued our research primarily on developing new methods for the analysis of research and power reactors. Through a bilateral agreement between the Slovenian Ministry and the CEA, we performed a series of measurements together with our French colleagues at the TRIGA reactor in Ljubljana to calibrate new, self-powered detectors and to measure the axial power distribution in the reactor using different methods. The results serve to improve the accuracy of our computational models, as well as neutron detectors; they improve the accuracy of the absolute thermal power calibration of the TRIGA reactor. Within the scope of another project with the CEA we tested and validated cross-section data for neutron dosimetry and neutron spectrum unfolding through activation measurements. The results were a contribution to the IRDFF library, which was recently released from the International Atomic Energy Agency (IAEA).



Asst. Prof. Andrej Trkov

Within the scope of our international activities we continued with the evaluation of nuclear data and their covariance matrices. We continued work on the evaluation of the data for manganese, we selected integral benchmark experiments for the validation of nuclear data for uranium-238 and the isotopes of iron; we also performed some sensitivity/uncertainty analyses for selected benchmarks within the OECD/NEA subgroup WPEC-33.

In the frame of the international collaboration (activities of the OECD/NEA Uncertainty Analysis in Modelling - UAM, WPEC SG33 and European Commission projects ANDES and F4E) we continued with the development of the methodology for the nuclear data sensitivity and uncertainty analysis. These methods were successfully

applied to fission reactors for reactor-safety studies (criticality, impact of delayed neutrons for reactor kinetics) as well as to future fusion-reactor (ITER) analysis. In the area of benchmark experiments we continued the long-term collaboration with ENEA Frascati in the FNG measurements and with OECD/NEA in the development of the SINBAD international shielding experiments database for fission, fusion and accelerators.

In the field of plasma physics we studied the formation of the potential in front of a negative electrode immersed in a plasma. Attention was focused on the analysis of the dependence of the floating electron emitting electrode on the electron emission. The problem was studied with PIC simulations of a plasma diode. The results were published in two scientific papers and in conference contributions. These results represent an important contribution to a better understanding of the use of emissive probes. We have shown that the saturation depends very much on the ratio between the temperature of the emitted electrons and the temperature of the basic electron population. If this ratio is low the floating potential indeed does not increase very much with increasing emission, after the temperature limited emission has been Figure 1: Neutron flux field in the JET torus; absolute value of the flux exceeded. For a larger ratio between both temperatures (above around 0.15) the floating potential continues to increase with increasing emission also



and its relative difference due to the presence of the remote-handling mascot robot during the neutron-source calibration.

above the temperature limited emission level and may even exceed the plasma potential. Our simulations explain the results of the measurements with emissive probes in low-temperature plasmas that have not been explained until now. We have continued our work on sheath formation in front of a negative electrode in a plasma in an oblique magnetic field. Attention was focused on a polytropic function and the deviation of the electron density from the Boltzmann distribution. Together with partners from Sofia university we also continued work on the interpretation of Langmuir probe I-V characteristics in magnetized plasmas.

In the field of **neutron-transport calculations** we continued and expanded our collaboration with JET – Joint European Torus, the largest fusion reactor in the world. Co-workers of the Reactor Physics Division have, in collaboration with JET staff, performed calculations of the neutron field inside the torus and in this way improved the understanding of the neutron detectors and their calibration. The work was necessary after the change of the torus first wall to beryllium during the last shut-down. The JSI staff is jointly responsible for the maintenance of the JET model for transport calculations with the Monte Carlo method and in 2012 our model was increased in detail, especially in the vicinity of diagnostics systems. The new model was also optimized for the calculation of correction factors, which are needed during the 2013 calibration.

We also collaborate on a project for neutron-detector calibration. Our tasks are transport calculations for the determination of calibration uncertainties and the determination of corrections, arising from the operating conditions, which differ from the conditions during calibration, e.g., in-vessel structures, neutron spectra, neutron source shape, etc. In 2012 our work was devoted especially to the remote-handling system and the analyses of its influence on the calibration of neutron detectors.

The work on the JET gamma camera was continued with a calculation of the neutron attenuation in the long version of the neutron attenuators, which will be used with the DT plasma. We calculated the neutron scattering locations inside the attenuator and improved the understanding of the noise due to scattered neutrons. In a similar way the intensity and location of the induced g rays, responsible for a lower quality of the measurements, was calculated.

Our research in the field of **medical physics** is directed towards image-guided cancer therapy. Within this general area, we were focused mainly on quantitative imaging with positron emission tomography (PET) with relatively new radiopharmaceutical 3'-Fluoro-3'-deoxythymidine (FLT), that is used for the imaging of cellular proliferation. Part of our work was more methodological, where we studied the quantification of FLT PET images with a kinetic analysis of FLT tissue uptake. The topic of this research was an optimization of the kinetic analysis method and an assessment of the kinetic analysis results' uncertainty. Through our collaboration with the University of Wisconsin (Madison, USA), we were involved in the planning and execution of clinical studies, where we used our kinetic analysis methodology for the assessment of radiopharmaceuticals tissue uptake. Besides that, we obtained some clinical data from the University of Wisconsin, which we used for a feasibility study of dose painting using a PET-based treatment response. In this study we found that such dose painting is feasible if the response is quantified with a robust metric (e.g., as a difference between two images FLT PET). The ratio of two FLT PET images, which would be the most straightforward extension already established definition of regional PET-based response, is at the application on voxel level severely affected with the imaging noise and therefore inappropriate.

Some outstanding publications in the past year

- 1. Gyergyek, T., Kovačič, J.: Saturation of a floating potential of an electron emitting electrode with increased electron emission: A one-dimensional kinetic model and particlein-cell simulation. Physics of Plasmas, 19, 2012, 013506.
- Popov, Tsv., Ivanova, P., Dimitrova, M., Kovačič, J., Gyergyek, T., Čerček, M.: Langmuir probe measurements of the electron energy distribution function in magnetized gas discharge plasma. Plasma Sources Sci. Techol. 21, 2012, 025004.
- Snoj, L., Žerovnik, G., Trkov, A.: Computational analysis of irradiation facilities at the JSI TRIGA reactor. Appl. radiat. isotopes. [Print ed.], 2012, vol. 70, pp. 483–488
- 4. Žerovnik, G., Trkov, A., Kodeli, I. A.: Correlated random sampling for multivariate normal and log-normal distributions. Nucl. instrum, methods phys res., Sect. A, Accel.. [Print ed.], 2012, vol. 690, pp. 75–78
- 5. Capote, R., Zolotarev, K., Pronyaev, V. G., Trkov, A.: Updating and extending the IRDF-2002 dosimetry library. Journal of ASTM International, 2012, iss. 4, vol. 9, p. 9
- Batistoni, P., Angelone, M., Fischer, U., Klix, A., Kodeli, I., Leichtle, D., Pillon, M., Pohorecki, W., Villari, R.: Neutronics experiments for uncertainty assessment of tritium breeding in HCPB and HCLL blanket mock-ups irradiated with 14MeV neutrons. Nucl. Fusion 52, 2012, 083014
- Kodeli, I., Snoj, L.: Evaluation and Uncertainty Analysis of the KRITZ-2 Critical Benchmark Experiments, Nucl. Sci. Eng. 171, 2012, pp. 231–238
- 8. Kirk, B. L., Grove, R. E., Kodeli, I., Gulliford, J., Sartori, E.: The current status of the shielding integral benchmark archive and database (SINBAD). Journal of ASTM International (JAI), Vol. 9, Iss. 3, p. 8, March 2012
- 9. Ivanov, K., Avramova, M., Kamerow, S., Kodeli, I., Sartori, E., Ivanov, E., Cabellos, O.: Benchmark for uncertainty analysis in modelling (UAM) for design, operation and safety analysis of LWRs, Volume I: Specification and support data for the neutronics cases (Phase I), Version 2.0, 2012
- 10. Gregoire, V., Jeraj R., Lee, J. A. and O'Sullivan, B.: Radiotherapy for head and neck tumours in 2012 and beyond: Conformal, tailored, and adaptive? Lancet Oncol 13(7), 2012, pp. e292–300
- 11. Vanderhoek, M., Perlman, S. B., Jeraj R.: Impact of the definition of peak standardized uptake value on quantification of treatment response. J Nucl Med 53(1), 2012, pp. 4–11

INTERNATIONAL PROJECTS

- Screening a selection of evaluations of structural materials for eventual anomalies to be signalled previous to the inclusion of the evaluations into the JEFF-32T2 test library Organisation for Economic Co-operation and Development Asst. Prof. Andrej Trkov
- Reports on thermal neutron induced SEU susceptibility of PXIe and cRIO fast controller components

ITER

- Dr. Luka Snoj
- 3. 7. FP EURATOM ANDES: Accurate nuclear data for nuclear energy sustainability European Commission
- Asst. Prof. Andrej Trkov 4. F4E - Action 2 -Nuclear data experiments and techniques ACTION F4E-GRT-056 (ES-AC) ACTION 2
 - European Commission
- Prof. Ivan Aleksander Kodeli
- 5. F4E-FPA-168-01; Nuclear data improvements and development of tools nuclear data evaluation
- European Commission
- Prof. Ivan Aleksander Kodeli
- FP EURATOM: public information; Research unit, administration and services RU-FU; Annex 3 to contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Acet. Deref. Auder: Televier.
- Asst. Prof. Andrej Trkov
- FP EURATOM: Upgrade of gamma-ray cameras: Neutron attenuators 2.2.1.- FU; EFDATask agreement JW6-TA-EP2-GRC-02, JW8-NEP-MHST-02 Ministry of Higher Education, Science and Technology Dr. Igor Lengar
- 8. Fusion Expo support action under EFDA work programme, task agreement WP10-PIN-FUSEX

Ministry of Higher Education, Science and Technology Dr. Igor Lengar

- 7. FP EURATOM; Improvement of diagnostic in edge plasmas of fusion devices 1.2.1.-FU; Annex 3 to contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Prof. Tomaž Gyergyek
- 7. FP EURATOM: Neutron calculations for fusion reactor-JET MCNP Model; 3.4.1.- FU; EFDA Task agreement JW9-FT-JET-5.32/JW9-NFT-MHST-03 Ministry of Higher Education, Science and Technology Dr. Igor Lengar
- 7. FP EURATOM: Neutron calculations for fusion reactor-neutron source 3.4.2.- FU; Annex 2 to contract 3211-08-000102; FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Dr. Luka Snoj
- 7. FP EURATOM; Neutron calculation for fusion reactor-JET MCNP MODEL 3.4.1.-FU11; Agreement TA JW11-FT-JET-5.36/JW11-NFT-MHST Ministry of Higher Education, Science and Technology Dr. Igor Lengar
- 7. FP EURATOM; Assessment of ANSYS workbench hybrid platform 4.10.1. FU; WP12-DTM-01-T03-01/MHEST/PS Ministry of Higher Education, Science and Technology Dr. Igor Lengar
- 7. FP EURATON; Neutronic studies for DEMO 4.10.2. FU Ministry of Higher Education, Science and Technology Dr. Igor Lengar
- 7. FP EURATOM; Emissive probes for AUG dlass tokamaks and beyond; WP12-IPH-A08-2-12/PS-01 Ministry of Higher Education, Science and Technology
 - Prof. Tomaž Gyergyek
- 7. FP EURATÓM; Measurements of SOL transport by probes in H-mode during ELM Intervals; WP12-IPH-A06-2-07/PS-01 Ministry of Higher Education, Science and Technology Prof. Tomaž Gyergyek
- 7. FP EURATOM, Measurements of SOL transport by probes in H-mode during Inter ELM Intervals; WP12-IPH-A06-1-1-07/PS-01 Ministry of Higher Education, Science and Technology Prof. Tomaž Gyergyek
- 7. FP EURATOM; He production-upper vertical port; WP12-DTM-04-T10-02/MHEST/PS Ministry of Higher Education, Science and Technology Dr. Igor Lengar

VISITORS FROM ABROAD

- 1. Prof. Giuseppe Gorini, University of Milano, Physics Department "G. Occhialini", Milan, Italy, 23.–24. 2. 2012
- Prof. Tsviatko Popov, Faculty for Physics, University "St. Kliment Ohridski", Sofia, Bulgaria, 14.–25. 5. 2012

- 7. FP EURATOM, MHEST Association; neutron calculation for fusion reactor, JET MCNP Model - 3.4.1.-FU, TA JW12-FT-JET, JW12-NFT-MHST Ministry of Education, Science and Sport Dr. Igor Lengar
- 7. FP EURATOM, MHEST Association; neutron calculation for fusion reactor, JET NEUTRON Sources Calibration - 3.4.2.-FU, TA JW12-FT-JET, JW12-NFT-MHST Ministry of Education, Science and Sport Dr. Luka Snoj
- 7. FP EURATOM, MHEST Association; neutron calculation for fusion reactor, upgrade of octant 1 JET MODEL - 3.4.3.-FU, JW12-FT-JET, JW12-NFT-MHST Ministry of Education, Science and Sport Dr. Igor Lengar
- 22. Improvement of evaluated nuclear data files with emphasis on activation and dosimetry reactions; Nuclear data libraries for advanced systems: Fusion devices (FENDL-3) IAEA - International Atomic Energy Agency
 - Asst. Prof. Andrej Trkov
- 23. Evaluation and validation of promt fission neutron spectra and the corresponding covariance matrices
 - IAEA International Atomic Energy Agency Prof. Ivan Aleksander Kodeli
- Feasibility study and installation of thermal neutron driven 14 MeV neutron converter into the TRIGA research reactor IAEA - International Atomic Energy Agency
- Dr. Luka Snoj 25. Research and development of plasma diagnostic techniques with emissive probe Slovenian Research Agency
- Prof. Milan Čerček 26. Evaluation and validation of the resonance parameters for structural materials Slovenian Research Agency Asst. Prof. Andrej Trkov
- Development and validation of procedures for propagation of uncertainties from the basic nuclear data to the integral reactor relevant parameters Slovenian Research Agency Prof. Ivan Aleksander Kodeli
- 28. Analyses of thermal power calibration method and joint experimental irradiation campaign at TRIGA research reactor Slovenian Research Agency
- Dr. Luka Snoj
- Development of an improved database for neutron spectrum characterisation in irradiation facilities of research reactors Slovenian Research Agency Asst. Prof. Andrej Trkov
- 30. Experimental verification of kinetic parameters of the TRIGA reactor and upgrade of the digital meter of reactivity Slovenian Research Agency Dr. Igor Lengar

RESEARCH PROGRAM

1. Reactor physics Asst. Prof. Andrej Trkov

R & D GRANTS AND CONTRACTS

- Functionalization of biomedical samples by thermodynamic non-equilibrium gaseous plasma Prof. Milan Čerček
- Calculations to support neutron monitor calibration JET fusion reactor example case Dr. Luka Snoj

NEW CONTRACT

- Expert opinion in Krško NPP tests and repairs during refueling at the end of fuel cycle 25 Milan Vidmar Electroinstitute Asst. Prof. Andrej Trkov
- Dr. Roberto Capote Noy, International Atomic Energy Agency, Vienna, Austria, 15.–27. 7. 2012
- 4. Dr. Christophe Domergue, CEA, Cadarache, France, 16.–20. 7. 2012, 3.–4. 10. 2012
- 5. Dr. Loic Barbot, CEA, Cadarache, France, 16.-20. 7. 2012, 3.-4. 10. 2012
- 6. Dr. Gwenole Corre, CEA, Cadarache, France, 16.–20. 7. 2012, 3.–4. 10. 2012
- 7. Dr. Mathieu Thevenin, CEA, Cadarache, France, 3.-4. 10. 2012

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- 10. Dr. Gašper Žerovnik
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12. Jernej Kovačič, B. Sc.

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- Duško Kančev, Gašper Žerovnik, Marko Čepin, "Uncertainty analysis in the nuclear industry: analytical unavailability modelling incorporating ageing of safety components", *J. loss prev. process ind.*, vol. 25, no. 3, pp. 643-649, 2012.
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- 18. JET EFDA Contributors: O. I. Kwon *et al.* (159 authors), "Stability analysis of high-beta plasmas in the Joint European Torus", *Plasma phys. control. fusion*, iss. 4, vol. 54, pp. 045010-1-045010-9, 2012.
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PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- 1. R. Capote, I. Konstantin, I. Zolotarev, V.G. Pronyaev, Andrej Trkov, "Validating the ENDF-B/VII 235U (nth,f) prompt fission neutron spectrum using updated dosimetry cross sections", In: *Proceedings PHYSOR 2012, Advances in reactor physics*, PHYSOR 2012, Advances in reactor physics, Knoxville, April 15-20, 2012, Knoxville, 2012, 7 pp.
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- 20. Luka Snoj, Žiga Štancar, Vladimir Radulović, Manca Podvratnik, Gašper Žerovnik, Andrej Trkov, L. Barbot, C. Domergue, Christophe Destouches, "Experimental power density distribution benchmark in the TRIGA Mark II reactor", In: *Proceedings PHYSOR 2012, Advances in reactor physics*, PHYSOR 2012, Advances in reactor physics, Knoxville, April 15-20, 2012, Knoxville, 2012, 15 pp.
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INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Luka Snoj, Borut Smodiš, "An analysis of a hypothetical terrorist action against a research nuclear reactor", In: *Managing the consequences of terrorist acts - efficiency and coordination challenges*, Denis Čaleta, ed., Paul Shemella, ed., Ljubljana, Institute for Corporative Security Studies, Monterey, Center for Civil-Military Relations, 2012, pp. 63-68.

MENTORING

- 1. Alberto Milocco, *Monte Carlo model for neutron production by the interactions of low energy deuterons in solid targets:* doctoral dissertation, Maribor, 2012 (mentor Andrej Trkov).
- Gašper Žerovnik, Use of covariance matrices for estimating uncertainties in reactor calculations: doctoral dissertation, Ljubljana, 2012 (mentor Andrej Trkov).

DEPARTMENT OF EXPERIMENTAL PARTICLE PHYSICS

Departmental research is devoted to experimental studies of elementary particles, to reveal the ultimate building blocks of matter and the nature of the interactions between them. Experiments are carried out within large collaborative programmes at international centres for particle physics at CERN near Geneva and at KEK in Tsukuba. The department is also engaged in developing and applying the technologically advanced particle detectors that are demanded by such measurements. Astroparticle physics is an emerging field applying the experimental techniques of particle physics to solve astrophysical problems. Slovenian researchers are participating in measurements of ultra-high-energy cosmic rays with the Pierre Auger observatory spread over a surface of 3000 km² near Malargue in Argentina.



In order to reveal the ultimate secrets of nature in the world of elementary particles, accelerators with higher and higher energies are needed. Their cost, both in terms of money and human resources, has grown to the level Head: where they are affordable only as joint international enterprises. Thus, future accelerators will be unique facilities Prof. Marko Mikuž of their kind, the first being the Large Hadron Collider (LHC), just completed at the European Organization for Nuclear Research (CERN) near Geneva. Researchers will exploit this facility to perform experiments in presently inaccessible regions of energy, which, though pushed higher and higher, still remains minute compared to that of the vast blast of the Big Bang that led to the creation of the Universe.

Together with colleagues from the Physics Department of the Faculty of Mathematics and Physics and the Faculty of Electrical Engineering of the University of Ljubljana, and from the Faculty of Chemistry and Chemical Technology of the University of Maribor, we are performing measurements at CERN and the Japanese centre KEK in Tsukuba. We are taking part in two experiments, each conducted as an international collaboration:

- ATLAS at the Large Hadron Collider (LHC) at CERN (3000 researchers, 174 institutions from 38 countries),
- Belle at the asymmetric electron-positron collider (KEK-B) at KEK (409 researchers, 62 institutions from 15 countries)

In the field of astroparticle physics we are part of the Pierre Auger collaboration (250 researchers, 94 institutions from 17 countries), which uses a giant scale (3000 km2) observatory near Malargue in Argentina for the detection of ultra-high-energy cosmic rays. This endeavour is carried out in collaboration with colleagues from the University of Nova Gorica.

A more detailed report on our 2012 activities follows, focused on the contributions of our researchers:

ATLAS experiment

Operation of the Large Hadron Collider LHC at CERN in 2012 exceeded the most optimistic expectations. The collision rate was increased by a factor of 2 compared to 2011 with stable operation even at the highest frequency. Two large experiments, ATLAS and CMS, had the opportunity to study collisions on a sample of integrated luminosity 23 fb⁻¹, 5 times larger than in 2011 and 500 times larger than in 2010.

The Slovenian group of ten scientists worked together with around 3000 colleagues in the ATLAS collaboration. A vast number of physical data analyses were made using global network Grid technology, in which the Slovenian capacities contributed a few percent of the data processing.

At a seminar held on 4 July 2012, the ATLAS experiment announced that it had observed a new particle: a boson consistent with the Higgs boson (Figure 1.). The excess of signal over background was observed at a mass

of around 126 GeV (Figure 2), and the level of confidence in the results was calculated to be 5 sigma. The possibility of a fluctuation of the background to this size of the signal is less than one in three and half millions (1,2). At the same seminar, ATLAS' sister experiment on the LHC, CMS, announced very similar results. The similarity acts as verification: if one experiment saw something very different to the other, there would be doubts about the results.

At a seminar held on 4 July 2012, the ATLAS experiment announced that it had observed a new particle: a boson consistent with the Higgs boson that has a mass of 126 GeV.

The news about the discovery of the Higgs boson was published in practically all the world's media. This result is an important advance in our understanding of the basic forces holding the Universe together. In particular this new boson provides support for the existence of the proposed Higgs field, which explains how some particles come



Figure 1: Event display of candidate for the decay of the Higgs boson into two muons and two electrons. Muon tracks are coloured red, electron tracks are coloured green. Tracks of other particles originating from twelve vertices are coloured orange.

to have mass and others do not. Without mass, all particles would fly around freely and matter as we know it would not exist. Physicists work to a theory of fundamental particles and their interactions called the Standard Model, which was first proposed in the 1970s. So far experiments have been able to confirm the existence of nearly all its elements with a high degree of precision. The Higgs boson, however, had eluded detection until now, prompting speculation that the theory could be incomplete. The findings so far suggest a Higgs boson compatible with the Standard Model, but further studies are needed to confirm this. We are looking for more Higgs particles which, according to almost all high-energy extensions of the Standard Model, should exist. Some of the most popular new models of physics are the so-called supersymmetry theories, which could potentially solve a number of problems in theoretical physics. The most minimalist supersymmetry theory predicts at least five (!) Higgs bosons: three neutral and two charged. So in the future if we detect more than one, we will know that we are looking at new physics!

The Slovenian group took a leading role in designing, building and operating the ATLAS Beam Condition Monitor (BCM), Beam Loss Monitor (BLM) and Radiation Monitor (RADMON). BCM, the more sophisticated system of the three, was built to monitor the conditions of the LHC beams

and issue warnings about unexpected and potentially dangerous situations. In 2011 and 2012 it acted as the ATLAS main luminosity monitor, reporting a great majority of almost 30 fb⁻¹, which were delivered to ATLAS. BLM, on the other hand, acted as a safety system and protected the ATLAS Inner Detector from potential damage by LHC beams, which fired and extracted LHC beams twice in the summer of 2011. RADMON records the doses received by different parts of the ATLAS Inner Detector.

A shutdown for more than a year is scheduled in 2013 and 2014. During this time, changes will be made to the collider to operate with increased energy and luminosity. The detector will also be upgraded to allow more accurate data taking. The most important change will be a new inner layer of silicon detectors (Inner B-layer – IBL). A special telescope tracker made of diamond detectors (Diamond Beam Monitor – DBM) constructed under the leadership of the Ljubljana group will be added in the region close to the beam pipe.

Belle detector at the asymmetric electron positron collider KEKB at KEK

The Belle detector at the electron-positron collider KEKB in Tsukuba, Japan, stopped taking data in 2010 in order to make room for an upgraded version of the detector. The new detector Belle II will begin operation in 2015. Meanwhile, the data collected by the Belle detector are still being used for a series of very interesting measurements. The main purpose of these measurements is the search for previously unknown particles and processes that are known as the New Physics. Among other things, such processes are responsible for the fact that we live in a universe in which matter (particles) completely dominates over antimatter (antiparticles).

In 2012, researchers of the Belle Collaboration (about 400 physicists from around the world) carried out so far the most accurate measurement of the parameter $\sin 2\Phi 1$, which describes the difference between particles and anti-particles (3). This measurement confirms with a high accuracy the theoretical predictions of M. Kobayashi

The Belle Collaboration carried out the most precise measurement of the parameter that describes the difference between particles and anti-particles, as well as a number of studies of rare processes in searches for New Physics. confirms with a high accuracy the theoretical predictions of M. Kobayashi and T. Maskawa, for which the two Japanese theoretical physicists shared the 2008 Nobel Prize for Physics. Slovenian physicists were leading a study where a new method was developed and applied to measure the probability of a decay of a charm meson to a pair of leptons, $Ds \rightarrow lv$ (4). This measurement is extremely difficult, as it is no spite of the improved method only possible to reconstruct one in 2000 events of this type. The result of

this precision measurement is consistent with the predictions of the Standard Model, the theory of interactions of elementary particles. In 2012, another important study was carried out, the measurement of the probability for a B meson decay into a tau lepton and its neutrino, $B \rightarrow \tau \nu$. This reaction is sensitive to possible contributions of a hypothetical charged Higgs boson, and resulted in restricting its mass to above 100 GeV/c².

In 2012, we continued with the preparation of the Belle II detector system. In this project, which includes almost 500 physicists from around the world, Slovenian colleagues play a key role, both in the management of the research group, as well as in developing new detection methods and methods for the analysis of the collected data.

Pierre Auger observatory

The Earth is exposed to a permanent rain of cosmic particles from outer space [1]. Most of the particles are fully ionized atomic nuclei, moving with relativistic energies. The bulk of them with energies up to 10^{17} eV originate

within our Milky Way. They are most likely accelerated in supernova remnants. Some particles have a thousand times higher energies, *i.e.*, around 10²⁰ eV. To clarify the origin of the highest-energy particles, their properties like energy, arrival direction and the particle type (photons, protons, atomic nuclei) have to be measured. The highest-energy cosmic rays are extremely rare. On earth one particle is registered in an area of 100 square kilometres in a

hundred years. The measurement of such particles requires a huge measurement device that is operated for a long time.

The Pierre Auger Observatory combines two complementary techniques to measure air showers. On their way through the atmosphere the secondary particles stimulate nitrogen molecules in the air to emit fluorescence light. This light is measured with large telescopes. In addition, secondary particles reaching ground level are registered in an array of particle detectors. The latter are water Cherenkov detectors, measuring the light emitted by relativistic particles passing through a water tank. The Pierre Auger Observatory is the largest-aperture cosmic-ray observatory at present, built to reach large statistics for the low flux of Ultra High Energy Cosmic Rays (UHECRs). Constructed in the province of Mendoza, Argentina, the observatory is the first hybrid air-shower experiment combining two independent observation techniques. It consists of 1660 water Cherenkov stations with 1.5 km spacing on a triangular grid (the surface detector, SD), overlooked by 24 fluorescence telescopes housed in four buildings (fluorescence detector, FD). It covers an area of 3000 square kilometres of Pampa and has a hexagonal footprint with a diameter of about 60 kilometres.

 Yes
 Selected diphoton sample

 0
 Data 2011+2012

 Sig+8kg Fit (m,=126.5 GeV)

 Bkg (4th order polynomial)

 4000

 1000

 15 = 7 TeV, Ldt = 4.8 fb⁻¹

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 1000

 110

 120

 130

 140

 150

 100

 100

 100

 110

 120

 130

 140

 150

 150

Figure 2: Measurement of photon pairs. The larger number of pairs around 126.5 GeV is indicating decays of the Higgs boson. Background is subtracted on the lower curve.

Above 10° eV, the cosmic ray flux falls with energy E roughly as E^{γ} where the spectral index γ -3. Several breaks in the spectral index have been observed reflecting cosmic ray properties like the interaction between particles and the photons of the 3K microwave background at 4×10¹⁸ eV and a fall-off at energies exceeding 10¹⁹ eV due to cosmic acceleration processes being proportional to the magnetic field in the astrophysical sources. Due to growing statistics every year an updated measurement of the energy spectrum is published. At the exposure of 5400 km² × sr × year a suppression with γ I = 2.59±0.02, γ Z = 4.3±0.02 and γ 3 = 4.3±0.02 was observed.

The identification of the type of the impinging cosmic-ray particle is experimentally the biggest challenge. Incoming particles such as atomic nuclei (of different masses), photons, and neutrinos induce cascades in the atmosphere. The longitudinal development of the showers depends on the particle type. Heavy nuclei interact early in the atmosphere, while light particles penetrate much deeper. This implies that for heavy nuclei the whole shower development takes place higher up in the atmosphere as compared to light particles. Thus, a measurement of the height of the shower above ground is a good estimate for the mass of the primary particle. Technically, we measure the distance between the detector and the position at which the shower contains its maximum number of particles. The investigations indicate that cosmic rays are composed of light particles (such as protons and helium nuclei)

at energies around 10¹⁸ eV. The data exhibit a trend towards heavier nuclei with increasing energy. At energies around 4×10^{19} eV, shower properties consistent with a heavy elemental composition (*e.g.*, silicon or iron nuclei) are observed [6]. At higher energies, at present, no mass measurement is available due to the small flux of particles at such energies. These mass measurements do assume that we can correctly extrapolate hadronic physics from accelerator experiments.

Searches for evidence of photons in the Auger event sets have resulted in no candidates. On the basis of this it is estimated that no more than a few per cent of all incident UHE messengers can be photons up to 30 EeV, with a weaker constraint at higher energies.

Given that the highest energy cosmic rays observed should exhibit trajectories that are relatively unperturbed by galactic and intergalactic magnetic fields, it is natural to wonder whether isotropy begins to emerge at these high energies. Furthermore, if the observed flux suppression is the GZK effect, there is necessarily some distance, (100 Mpc), beyond which cosmic





Figure 3: The mass distribution of the reconstructed D_s meson decays $D_s \rightarrow \mu v$. For this measurement, a novel method was developed, which leads a large number of correct reconstructions (peak in the distribution) (4).

the measurement of the arrival times of the individual particles at the surface detectors allows us to measure the shower disc, with the arrival direction being perpendicular to it. Based on the Auger data set, 28 out of 84 events with energies higher than 5.6×10^{19} eV were found to be correlated with objects in the Veron-Cetty catalogue of active galactic nuclei. The overall correlation strength thus decreased from $(62 \pm 10)^{\%}$ previously published to $(33 \pm 5)^{\%}$. However, the chance probability of observing such a correlation from a random distribution remains below 1%. Correlations on such a small angular scale as those reported (3.1°) would seem to be at odds with the apparent trend to heavy compositions at high energy, since heavier nuclei would be more deflected by intergalactic and galactic magnetic fields.

Detector development

In 2012, we continued the development of new methods for the detection of annihilation gamma rays in positron emission tomography (PET), one of the most important medical imaging methods. If a Cherenkov radiator is used as a gamma-ray converter instead of a scintillator, the difference in the time of flight of the two gamma rays can be measured with a very high precision of 80ps (FWHM). In this way we can directly obtain three-dimensional information on the emission point of the two gamma rays, which substantially reduces the time needed to determine the activity distribution in the patient. We have also developed a new method for the detection of gamma rays with a scintillator in which the depth of the gamma-ray conversion within the crystal is determined from a ratio of signal intensities in the neighbouring detector pixels. In 2012, the much awaited comprehensive publication "Handbook of particle detection and imaging" was published, for which we have contributed a chapter on the detection of photons in an elite company of the greatest experts for detectors in particle physics (5).

The development of radiation hard silicon detectors is very important for future high-energy experiments. We used innovative edge-TCT method, developed at our laboratory, to measure the electric field in silicon detectors. Detectors were irradiated at the nuclear reactor in Podgorica near Ljubljana with neutrons up to fluences of 5×10^{16} cm². Changes in the electric field during annealing were recorded and explained.

As part of the CIMA collaboration dedicated to developing new instrumentation methods for imaging in Nuclear Medicine we extended the high-resolution PET probe prototype built at the University of Michigan with silicon detectors segmented into cubic cells with a side of 1 mm. This

halved our measurement precision, which was reflected in recorded images of nuclear medicine phantoms filled with the F-18 isotope. A new data-acquisition system (MADDAQ) was completed and tested. In the scope of the development of new detector solutions we constructed the first module based on flex-rigid circuit connecting the detector cells to the front-end readout electronics and continued the testing of samples of interpolating pad silicon detectors.

We performed more than 100 irradiations at Nuclear Reactor Podgorica in the framework of AIDA (Advanced European Infrastructures or Detectors at Accelerators) for 15 interested institutions. In the second year of this project the emphasis was on upgrades for the ATLAS, CMS and BELLE detectors.

Organization of Conferences, Congresses and Meetings

- 1. 7th "Trento" Workshop on Advanced Silicon Radiation Detectors (3D and P-type Technologies) Jožef Stefan Institute, Ljubljana, Slovenia; 29. 2. 2. 3. 2012
- 2. "ATLAS Production System Meeting", Jožef Stefan Institute, Ljubljana, Slovenia, 20. 6. 2012 22. 6. 2012

Awards and Appointments

- 1. Zois Award for Special Achievements in Particle Physcis, Prof. Dr. Boštjan Golob, Prof. Dr. Samo Korpar, Prof. Dr. Marko Starič
- 2. Puh award for invention of intelligent motor drives of valves, Aleš Svetek, M.Sc.
INTERNATIONAL PROJECTS

- Design, procurement and QA of flex-rigid hybrids 1. European Organization for Nuclear Research Prof. Marko Mikuž
- Scanning transient current technique (S-TCT) 2. Vizus, d. o. o. Dr. Gregor Kramberger
- 7. FP RADDOS: Joint research on various types of radiation dosimeters 3. European Commission
- Dr. Gregor Kramberger
- 7. OP MC-PAD: Marie Curie training network on particle detectors; PITN-GA-2008-214560 European Commission
- Prof. Peter Križan
- 7. FP IMPACT: Improving access to text 5. European Commission Jan Jona Javoršek, B. Sc.
- 6. FP - EGI-InSPIRE: European grid initiative: integrated sustainable pan-European infrastructure for researchers in Europe European Commission
 - Prof. Marko Mikuž
- FP AIDA: Advanced European infrastructures for detectors at accelerators European Commission Prof. Marko Mikuž
- FP HadronPhysics3: Study of strongly interacting matter European Commission
- Prof. Samo Korpar
- FERRO-PATCH: Frequency and polarisation agile microstrip patch antenna based on ferrelectric varactors ESA/ESTEC
 - Prof. Vladimir Cindro
- 10. Development of new detectors for PET imaging Slovenian Research Agency Prof. Marko Mikuž
- 11. Development of silicon and diamond semiconductor detectors for particle physics experiments and medical imaging Slovenian Research Agency
- Dr. Andrei Gorišek 12. Doping of semiconductor nanocrystals by neutron transmutation method (NTD)

Slovenian Research Agency Asst. Prof. Igor Mandić

RESEARCH PROGRAMS

- Astroparticle physics 1
- Prof Marko Zavrtanik 2
- Experimental particle physics Prof. Marko Mikuž

R & D GRANTS AND CONTRACTS

- Measurements of mixing and CP symmetry violation in D^0 meson system 1. Prof. Boštjan Golob
- 2 Gridification of particle physics data analysis: a pilot project of Slovenian National Grid Initiative
- Prof. Marko Mikuž
- Particle detectors at future generation colliders 3 Prof. Marko Mikuž
- Development of solid state detectors for particle physics experiments
- Prof. Vladimir Cindro 5 Workshop on advanced silicon radiation detectors (3D and P-type technologies) Dr. Gregor Kramberger
- Measurement of the absolute branching fractions of leptonic D(s) decays and the extraction of the decay constant $f_D(s)$
- Dr. Anže Zupanc Collaboration CERN RD-39
- Prof. Marko Mikuž Collaboration CERN RD-50
- Prof. Marko Mikuž
- 9 Collaboration ATLAS Prof. Marko Mikuž
- Collaboration CERN RD-42 Prof. Marko Mikuž
- 11 Collaborations Belle in Belle II Prof. Peter Križan
- 12. Collaboration CIMA: cameras for imaging in medical applications Prof. Marko Mikuž

VISITORS FROM ABROAD

- 1. Dr. Ivana Capan, Ruđer Bošković Institute, Zagreb, Croatia, 11. 4. 14.4.2012
- 2. Dipl. ing. El. Miomir Todorović, University of Niš, Niš, Serbia, 1. 4. - 23. 4. 2012
- 3. Dr. Adrian Bevan, Queen Mary College London, London, UK; Dr. Bruce Yabsley University of Sydney, Sydney, Australia; Prof. Dr. Soeren Prell, University of Iowa, Iowa, USA; Prof. Dr. Thomas Mannel, University of Siegen, Germany, 18. 5. - 25. 5. 2012
- 4. Dr. Shohei Nishia, KEK, Tsukuba, Japan, 18. 7. - 22. 7. 2012
- Prof. dr. Carl Wilhelm Eduard Van Eijk, Technical University DELFT, Netherlands, 12. 5. 9. - 14. 9. 2012
- 6. Dipl. ing. El. Miomir Todorović, University of Niš, Niš, Serbia, 2. 10. - 23. 12. 2012

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- 42. Andreja Butina
- 43. Jurij Eržen

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ORIGINAL SCIENTIFIC ARTICLE

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- Matej Batič, M. Han, S. Hauf, Gabriela Hoff, C. H. Kim, M. Kuster, Maria Grazia Pia, Paolo Saracco, H. Seo, "Algorithms and parameters for improved accuracy in physics data libraries", In: *Proceedigs of the International Conference on Computing in High Energy and Nuclear Physics 2012 (CHEP2012), 21-25 May 2012, New York, USA*, (Journal of physics, Conference series, vol. 396, no. 1/6, 2012), Bristol, Institute of Physics Publishing, 2012, vol. 396, no. 2, pp. 022039-1-022039-7, 2012.
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- AUGER Collaboration: L. Cazon *et al.* (505 authors), "Studying the nuclear mass composition of Ultra-High Energy Cosmic Rays with the Pierre Auger Observatory", In: *12th International Conference on Topics in Astroparticle and Underground Physics (TAUP 2011), 5-9 September 2011, Munich, Germany*, (Journal of physics. Conference series, vol. 375), George Raffelt, ed., L. Oberauer, ed., R. M. Wagner, ed., Bristol,

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INDEPENDENT SCIENTIFIC COMPONENT PART OR A Chapter in a Monograph

- 1. Peter Križan, "Photon detectors", In: *Handbook of particle detection and imaging.* 1, Claus Grupen, ed., Irène Buvat, ed., Berlin, Heidelberg, Springer, 2012, zv. 1, pp. 297-311.
- 2. Dejan Žontar, "Radiation doses from patients to staff members, comforters and caregivers and to the general population", In: *Radiation protection in nuclear medicine*, Sören Mattsson, ed., Christoph Hoeschen, ed., Heidelberg [etc.], Springer, 2012, pp. 109-128.

MENTORING

- 1. Rok Dolenec, *Time-of-flight positron emission tomography using Cherenkov radiation:* doctoral dissertation, Ljubljana, 2012 (mentor Samo Korpar).
- 2. Borut Grošičar, *Development of detectors for high resolution positron tomography:* master's thesis, Maribor, 2012 (mentor Samo Korpar; comentor Vladimir Cindro).

DEPARTMENT OF INORGANIC CHEMISTRY AND TECHNOLOGY K-1

The Department of Inorganic Chemistry and Technology is one of the leading groups in the field of the synthesis of new inorganic compounds containing fluorine in the world. The main research fields are the synthesis of new coordination compounds with different ligands, the chemistry of noble gases, the chemistry of elements of the main groups and the synthesis of new inorganic materials with special properties. A great deal of the activity of the group has been devoted to technological, ecological and safety problems in Slovenia. The group has already been cooperating closely with Slovenian industry for more than thirty years. It is also active in the field of education and in the field of the promotion of natural sciences among students at colleges and elementary schools.



The chemistry of noble gases represents an important part of the research activities of the department. The 50th anniversary of the discovery of the first true noble gas compound - xenon hexafluoroplatinate(IV) is marked this year. Despite a number of theories and speculations about its nature, the structure of this compound remains unknown. Certain syntheses and partial characterizations of these types of compounds, with a general formulation XeF, MF, were carried out several years ago, but most of their crystal structures were left unsolved. The focus of Asst. Prof. Gašper Tavčar our research was the system XeF₂/TiF₄, and we successfully synthesized and fully characterized three new compounds: (XeF)₂Ti₂F₁₀·XeF₂, Xe₂F₃Ti₈F₃₃ and (XeF)₂Ti₉F₃₈. The formation of the compound Xe₂F₃Ti₈F₃₃ represents the first synthesis of a Xe₂F₃* salt without using excess XeF₂ and it is the first known Xe₂F₃* salt in the systems XeF₂/MF₄* This compound probably reacts further on with an additional TiF_4 to give the salt (XeF), Ti_0F_{20} , where a nonameric

 $[Ti_{0}F_{20}]^{2}$ anion has been observed for the first time. A distinguishing feature of these two compounds is their unusually high thermal stability - both are stable for longer periods at higher temperatures (~100°C). Work on the VOF_a/XeF_a system yielded the XeF_a 4VOF_a compound, a rare example of an interaction between a Lewis base XeF, and a Lewis acid metal oxyfluoride.

We have continued with the study of the coordination properties of XeF, connected as a ligand to a metal centre. We synthesized and structurally characterized $[Li_2(XeF_2)](V_2O_2F_8)$, which is the second example of a compound in which XeF_a acts as a ligand towards the Li⁺ cation and several structurally diverse compounds with the Hg²⁺ cation: $[Hg(XeF_{2})_{2}](AsF_{6})_{2}, [Hg(XeF_{2})_{2}](AsF_{6})_{2}, [Hg(XeF_{2})_{2}](SbF_{6})_{2} and [Hg_{2}(XeF_{2})_{6}](SbF_{6})_{4}. We continued our collabora$ tion with the McMaster University, Canada, on the coordination chemistry of kripton difluoride.

The synthesis and characterisation of new inorganic compounds with fluoridomonooxidovanadium(V) anions

was continued. With a systematic investigation of the reactions between various metal fluorides and VOF, in an anhydrous hydrogen fluoride solvent we wanted to prepare new anionic vanadium oxyfluorides and understand what affects the type of anions formed in these reactions. This knowledge is crucial for the design and selective syntheses of materials with the desired dimensionality of oxyfluoro anions. The ratio between vanadium trifluoride oxide and fluoride anions in the solution has proven to be an important factor influencing the type of anion formed. With adjustments of this ratio we were able to isolate two new representatives of this compounds in the lead and rubidium systems, i.e., Pb[VOF_c] with monomeric and Rb[VOF₄] with polymeric chain anion. A similar polymeric anion was also observed in the case of a silver compound - Ag[VOF₄]. In collaboration with the University of Ljubljana we have begun to investigate how structures of fluoridomonooxidovanadium(V) anions are affected by organic cations formed in anhydrous HF from various amines, such as DABCO (1,4-diazabicyclo[2.2.2]octane).

Reactions between alkaline metal fluorides (MF; M = Li, Na, K, Rb, Cs) and TiF, in an anhydrous hydrogen fluoride solvent were investigated. The crystal structures of Rb_2TiF_6 , $CsTiF_5$, $MTiF_5$ HF (M = Na, K, Rb), NaTi₂F₉ HF, $K_4[Ti_8F_{36}]$ ·8HF and $Rb_4[Ti_8F_{36}]$ ·6HF were determined. Most interesting are the Figure 1: TiF_6 octahedra forming the $([Ti_8F_{33}]^-)_n$ polyanion and the

Prof. Boris Žemva received a Mentor of the Year Award from the Society of Young Researchers of Slovenia



crystal structures of the latest two. They consist of alkaline metal cations, arrangement of planar Xe, F, units in the structure of Xe, F, Ti, F, 3



Figure 2: Basic building unit of the XeF, 4VOF, crystal structure.

neutral HF molecules and octameric $[Ti_8F_{36}]^4$ anions. Each $[Ti_8F_{36}]^4$ anion is made from eight TiF_6 octahedra, which are arranged in such a way that the central Ti atoms are placed on the vertexes of a virtual cube. In this way each TiF_6 shares three apexes with three neighbouring TiF_6 units.

The dissolution of oxides MO (M = Zn, Cu, Hg) in superacid aHF/AsF_5 or the reaction between H₃OAsF₆, FeF₂ and AsF₅ in aHF as a solvent yield H₃OM[AsF₆]₃ (M = Fe, Zn), H₃OMF[AsF₆]₂ (M = Fe, Cu) and (H₃O)₂Hg₃F[AsF₆]₅.

The $[CF_3SO_3]$ anion is found in nearly seven thousand crystallographically characterized compounds and in myriads of others that have not been analysed with structural methods. Among all such inorganic compounds the silver(I) derivative (AgSO_3CF_3) is the most frequently utilized in chemical synthesis. The reason is in its excellent solubility in water and in a broad spectrum of organic solvents; on the other hand, the corresponding chloride, bromides and iodides are insoluble in these media. This difference in solubility is the main force in many metathetic (ligand exchange) reactions where the precipitation of silver(I) halogenides and the incorporation of SO_3CF_3 species in desired compounds occur. In cooperation with the University of Warsaw we have investigated the physicochemical properties of AgSO_3CF_3 and AgSO_3F. Their crystal structures were also determined and their thermal decompositions investigated.

In cooperation with Ukrainian partners (Lvov university) we have investigated the structural properties of copper (I) pi-complexes. Isomer-selective coordination in the case of allylbenzotriazole isomers was observed in $CuBF_4 \times 2$ -all-bta $\times H_2O$, $CuClO_4 \times 2$ -all-bta, $CuClO_4 \times 1$ -all-bta $\times 2$ -all-bta and $CuHSO_4 \times 2$ -all-bta compounds. Anion-depending coordination was observed in $[Cu(\eta_2 C_{10}H_{10}SN_2)(C_7H_6SN_2)NO_3]$ and $[Cu(C_7H_6SN_2)_2]ClO_4$.

Within the research on the heterogeneous reactions of trifluoromethane with some metal oxides at relatively low temperatures it was found that the acidity of fluorinated mixed oxides based on γ -Al₂O₃/ γ -Ga₂O₃ in addition to the extent of fluorination decisively depends also on the gallium content. This was attributed to the preferential

Octahedral units of [TiF₆] in the compounds could be isolated or linked by sharing vertexes, edges and faces. In this way in these compounds larger polyanions such as isolated cube, infinite chains (1D), layers (2D) or three-dimensional networks are formed. replacement of the most acidic surface Al³⁺ ions with less acidic Ga³⁺ ions. Such a replacement of ions in mixed oxides leads to an unproportionate formation of acidic sites with lower strength. With the appropriate Al/Ga ratio and partial fluorination, solid materials with tailored acidity can be prepared.

 as isolated cube, infinite
 Research of aerogels based on aluminium(III) fluoride was continued.

 2D) or three-dimensional networks are formed.
 Work in this field was focused on the determination of surface characteristics and on the nanostructure of this new class of materials. The latter investigations showed that fluoride aerogels consist of relatively uniform anisotropic nanoparticles that in turn consist of amorphous and distinctive nanocrystalline phases.

Molybdenum nitride with 11 m²/g of specific surface area was synthesized by nitriding the coordination compounds CpMoCl₄ and Mo(CO)₄(bipy) (Cp=cyclopentadienyl, bipy=2,2'-bipyridine) for the purpose of the preparation of new catalysts with improved properties for the ammonia synthesis process. Molybdenum disulphide with 24 m²/g of specific surface area was prepared by the reaction of CpMoCl₄. Mo(CO)₄ and MoCl₅ with H₂S gas and the

reaction conditions were optimized for the maximum value of the specific surface area. Synthesized molybdenum disulphide is catalytically active for the synthetic gas reaction, where the products are methane and water. Three new coordination compounds with the $[Mo_2O_4F_6]^2$ anion were synthesized and their structures determined by single-crystal X-ray diffraction.

Thermodynamic and kinetic effects during a pH titration of As(III) in the buffered malonate system with iodine were investigated. Classic and pHstatic titration approaches were comparatively studied for the Liebig–Denigès method of cyanide determination. Experiments on the contents of fluorine taken up by nettle from fluoride contaminated soil were conducted. The results indicate that nettle is remarkable bioaccumulator of fluoride from soil. As result, nettle could be suggested as a promising phytoremediator for fluoride contaminated soil.

The project "Speciation and interactions of chemical contaminants at trace level in aqueous media to support the development of cost effective removal technologies" in cooperation with the department O2 is progressing as planned, with the development and experimental confirmation of theoretical



Figure 3: Infinitive chains of polyanions $([TiF_5]^-)_n$ in the structure of $KTiF_5$ -HF

modelling findings as a part of the catalytic oxidation of mercury chemistry research in the wet flue-gas desulphurisation processes. The partners in the 3-year project are the departments O2, K1 and the University of Maribor. The project co-workers prepared an article that was accepted for publication in the Fuel magazine, and the results were attracting interest at several scientific and professional conferences.

In the field of environmental and social impact assessments two coworkers of the department joined the EU FP7 project CiViTAS ELAN in the roll of evaluators of four (of a total of sixteen) measures under implementation in Ljubljana and in the partner cities of Ghent, Porto, Brno and Zagreb. The aim of these measures is to improve the quality and safety of the public and private users' mobility. Special emphasis is given to the efficiency analysis of the implemented measures, focused on the activities during the European Mobility Week in September 2012, when Ljubljana city centre was closed to private motorised traffic. The project successfully finished in October 2012 with a line of improvement in the public mobility in all participating cities. The improvement is not finished with the closing of the project, because one of the main objectives of the project was the modern approaches towards raising the public transport users' and service providers' awareness, so the mobility improvement measures are mirroring in other cities, and some long-term measures like the construction of P&R at the entrances to the city along with the implementation of dedicated public transport "yellow" lanes, enlargement of pedestrian-only zones

In the EU FP7 project Integ-Risk we continued our work on the key performance indicators on the quality for mutual consideration of the process safety-risk assessment and spatial planning process. We led the testing of some methods and tools for the management of new and emerging risks in industry. In that respect we tested in the industrial zone of Luka Koper (Port of Koper), Slovenia and in the Industrial Zone Pančevo, Serbia, methods for: i:) analysing risks between the client and contractors, ii.) an approach to the selection of the key performance indicators (applied to the process safety), iii.) an approach to the analysis of the energy supply security, iv.) an approach to the assess-



Figure 4: TEM images of an AlF₃-based aerogel show that in these materials some ordering already takes place. Anisotropic nanosized basic particles consist of distinct crystalline and amorphous phases. (Images: D. Primc, K-8)

The EU FP7 Project CiViTAS ELAN was successfully completed. One of the main goals of the project was raising the awareness of users and service providers about modern approaches to mobility in cities.

ment of the health effects due to exposure to hazardous substances, v.) the domino accident potential among two industrial establishments, vi.) a tool for the spatial integration of the risk information (process safety aspect) and vii.) an approach to consider the risk information within the process of land use planning/plan elaboration (at the local community level).

(including the closing of a part of Slovenska Road) and others, are planned for implementation in 2013 and beyond

In October 2012 we started an IPA project Adriacold "Diffusion of cooling and refreshing technologies using the solar energy resource in the Adriatic regions", along with partners from Italy, Slovenia, Croatia, Bosnia &

Hercegovina and Albania. We cooperate in several project work tasks, and led the work task "Monitoring and data mining", including the planning, systematic collection of performance data of five pilot and testing cooling plants (in the cities of Dubrovnik and Rijeka (Croatia), Piran (Slovenia), Dolina and Rimini (Italy)), and data analysis. The project will include a public tender for the installation and testing of sustainable cooling facilities, in which Slovenian industry that develops and markets such equipment can participate and benefit.

We also joined the Razvojni center Energija d.o.o. (RCE) project "Methodology of fixation of CO₂ on fly ash", where the department researchers provide consulting and support work for the technology development on the pilot and semi-industrial scale based on laboratory-test findings.

The activity in the field of education and the promotion of sciences should be mentioned. Five co-workers were actively engaged in the work of the Jožef Stefan International Postgraduate School as lecturers and as mentors to M.Sc. and Ph.D. students. In addition, the School of Experimental Chemistry maintained its very important relations with elementary, secondary schools and even kindergartens through experimental courses performed in a specialised laboratory or through direct demonstrations at the schools.



Figure 5: Quadrupole mass spectrometer HiQuad manufactured by Pfeiffer was installed and tested. Mass spectrometer was partly funded by the ARRS through the "Oprema XIV" call and is configured for the analysis of gaseous samples at up to 1 bar pressure.

A part of these activities is included in the European project KidsINNscience (the project will be finished in 2013) in which eight partners from Europe and two from Latin America participate. New methods for learning natural sciences were tested. With demonstrations of chemical experiments we participated at the 18th Slovenian Science Festival, organized by the Slovenian Science Foundation, at the 5th Science Festival organized by the Centre for Youth Culture, at the Researchers night in Ljubljana and on the television show "Ugriznimo znanost" (Bite the science).

Some outstanding publications in the past year

- 1. Grochala, W., Ksawery Cyránski, M., Derzsi, M., Michałowski, T., Malinowski, P., Mazej, Z., Kurzydłowski, D., Koźmiński, W., Budzianowski, A., Leszczyński, P. J.: Crystal and electronic structure, lattice dynamics and thermal properties of Ag(I)(SO₃)R (R = F, CF₃) Lewis acids in the solid state. Dalton Trans., 2012, 41, pp. 2034–2047
- 2. Koblar, A., Tavčar, G., Ponikvar-Svet, M.: Fluoride in teas of different types and forms and the exposure of humans to fluoride with tea and diet. Food Chem., 2012, 130, pp. 286–290
- Blinc, R., Cevc, P., Tavčar, G., Žemva, B., Laguta, V., Trontelj, Z., Jagodič, M., Pajić, D., Balčytis, A., Scott, J. F.: Magnetism in multiferroic Pb₅Cr₄F₁₀, Phys. Rev., B, Condens. Matter Mater. Phys., 2012, 85, 054419-1 - 054419-5
- 4. Mazej, Z., Goreshnik, E. A., Jagličić, Z.: Syntheses and crystal structures of [H₃O]^{*}/M^{2*} (M = Fe, Zn, Cu, Hg) salts with [AsF₂]; European J. Inorg. Chem., 2012, pp. 1734–1741
- 5. Valkulka, A., Tavčar, G., Skapin, T.. Interaction of trifluoromethane (CHF₃) with alkali hydroxides and carbonates. J. Fluorine Chem., 2012, 142, pp. 52–59

Awards and appointments

1. Prof. Boris Žemva: Award for Mentor of the Year 2012, given by the Young Researchers Association of Slovenia.

Patent granted

1. Adolf Jesih, Andrej Kovič, Aleš Mrzel, Method for a synthesis of quasi-one-dimensional structures of 4d and 5d (Nb, Mo Ta, W) transition metals, SI23768 (A), Urad RS za intelektualno lastnino, 31.12.2012.

INTERNATIONAL PROJECTS

- Analyses of the Soluble Parts of the Catalyst Porzellanfabrik Frauenthal Gmbh Asst. Prof. Gašper Tavčar
- 7.FP CIVITAS-ELAN; Mobilising Citizens for Vital Cities Ljubljana-Gent-Zagreb-Brno-Porto European Commission Asst. Prof. Marko Gerbec
- 7. FP iNTeg-Risk; Early Recognition, Monitoring and Integrated Management of Emerging, New Technology Related Risks
- European Commission Asst. Prof. Marko Gerbec
- 4. 7. FP KidsINNscience; Innovation in Science Education Turning Kids on to Science European Commission
- Tomaž Ogrin, M. Sc.5. ACT CLEAN Access to Technology and Know-how in Cleaner Production in Central Europe European Commission
- Dr. Andrej StergaršekDiffusion of Cooling and Refresing Technologies using the Solar Energy resources in the Adriatic Regions
 - Consorzio per l'AREA di ricerca Scientifica Asst. Prof. Gašper Tavčar
- COST ES1006; Evaluation, Improvement and Guidance for the Use of Local-scale Emergency Prediction and Response Tools for Airborne Hazards in Built Environments COST Office Asst. Prof. Marko Gerbec

VISITORS FROM ABROAD

 Prof. Joel F. Liebman, Department of Chemistry and Biochemistry, University of Maryland, Baltimore, USA, 26. 3.–1. 4. 2012

- Selective Synthesis of Fulerenic Superhalogens and Flurinated Superweak Anions Slovenian Research Agency Prof. Boris Žemva
- Tungsten Carbide: Fine Powders Obtaining and Coatings Deposition from Melts, Regeneration from Industrial Wastes Slovenian Research Agency Dr. Melita Tramšek

RESEARCH PROGRAM

1. Inorganic Chemistry and Technology Asst. Prof. Gašper Tavčar

R & D GRANTS AND CONTRACTS

- Speciation and interactions of chemical contaminants at trace level in aqueous media to support the development of cost-effective removal technologies Dr. Andrej Stergaršek
- Optimisation of a polychlorinated biphenyls' (PCBs) contaminated material dump site remediation Dr. Andrej Stergaršek
- Expert opinion, attendance at the expert meeting and presentations for the aspects of major accident prevention and Mercury pollution in the Gulf of Trieste Asst. Prof. Marko Gerbec
- Dr. Angelina Gab, Dr. Dmytro Shakhinin, National Technical University of Ukraine, Ukraine, 27. 11.–4. 12. 2012

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- Asst. Prof. Evgeny Goreshnik
 Dr. Adolf Jesih
- Asst. Prof. Robert Kocjančič

- 5. Dr. Zoran Mazej
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- Dr. Andrej Stergarsek, rettred 02.12.1
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 Gleb Veryasov, B. Sc.

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 $[C_2H_4N_2(CH_3)_4(C_3H_5)_{2_{0.5}}Cu_2Cl_{1.67}Br_{1.33}]", \textit{J. struct. chem., vol. 53, no. 1, pp. 119-124, 2012.}$

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INDEPENDENT SCIENTIFIC COMPONENT PART OR A

CHAPTER IN A MONOGRAPH

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PATENT APPLICATION

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- 2. Andrej Kovič, Adolf Jesih, Aleš Mrzel, The procedure for the synthesis of 4d and 5d (Nb, Mo Ta, W) nitrites of transition metals in the form of quasi-one-dimensional structures, P-20120057, Urad RS za intelektualno lastnino, 22.2.2012.

PATENT

1. Adolf Jesih, Andrej Kovič, Aleš Mrzel, *Method for a synthesis of quasione-dimensional structures of 4d and 5d (Nb, Mo Ta, W) transition metals*, SI23768 (A), Urad RS za intelektualno lastnino, 31.12.2012.

MENTORING

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DEPARTMENT OF PHYSICAL AND **ORGANIC CHEMISTRY** K-3

The basic research of the department is focused on the experimental and theoretical study of various physico-chemical processes at surfaces and in atmospheric chemistry. The main attention in the field of organic chemistry is directed to the halogenated, in particular fluorinated, organic molecules.

Experimental research in the field of electrochemistry continues for the materials that are important in industrial and biomedical applications. The corrosion protection of alloys used in these applications can be achieved by various treatments - from surface layers to functional modifications of the surface and corrosion inhibitors. Materials of interest are alloys based on iron, aluminium, copper, zinc and magnesium, as well alloys based on titanium and cobalt. Within the project Surfuncti financed by the European Research Area (ERA) we have investigated a novel alloy for biomedical applications, Ti-20Nb-10Zr-5Ta. Compared to commercial Ti-based alloys the novel alloy exhibits better mechanical properties, i.e., lower elastic modulus and higher hardness, being at the same time more corrosion protective under simulated physiological conditions. In terms of biocompatibility, the Head: novel alloy performs similar to titanium. The project was performed in collaboration with the Institute of Physical Prof. Ingrid Milošev Chemistry "Ilie Murgulescu" from Bucharest and the Faculty of Health Sciences University of Primorska. We have continued our studies on the biomedical alloy Nitinol, which exhibits two closely related and unique properties: shape memory and super-elasticity. The corrosion properties of this alloy are not satisfactory under certain conditions due to the high content of nickel, whose corrosion resistance is poor. While in our previous studies we have shown that the corrosion stability of Nitinol can be improved by the low-temperature oxidation in water and high-temperature oxidation in air, we have also tested other procedures like anodic oxidation and self-assembling. By anodic oxidation in acetic acid the TiO, oxide layer is formed at the surface. concentration / at This layer contains only a few percent of NiO, which is important since nickel is a known allergen and its content should be kept at a minimum. A promising method for the functional modification of the surface is the self-assembling procedure. In collaboration with the Faculty of Chemical Engineering and Technology from the University of Zagreb we have investigated the possibility of changing the interface structure and surface chemistry of the Nitinol surface using octadecylphosphonic acid. A self-assembled covalently bonded (monodentate type) film of octadecylphosphate is formed, which effectively protects the surface 8 of Nitinol under simulated physiological conditions.

When investigating the materials to be used for biomedical applications it is desirable to mimic closely the conditions in vivo. Various simulated physiological conditions are normally used for in-vitro studies; however, these solutions cannot completely simulate in-vivo conditions. One of the most important differences is the presence of various biologically active organic species. In orthopaedic applications the natural environment of the metal implant is the synovial fluid in the joint. The effect of synovial fluid on the formation, composition and thickness of the layer formed at the surface of the CoCrMo alloy in various simulated physiological solutions was investigated in detail. The addition of synovial fluid significantly hinders the formation of the oxide layer and reduces the formation of the calcium phosphate layer.

The formation of various coatings on the surface of metals and alloys is another way of corrosion protection for technologically important materials like aluminium and its alloys. Due to their beneficial properties, aluminium and its alloys are used in numerous applications in civil engineering, the automotive and aerospace industries, food and the electronics industry. These materials exhibit low density, high tensile strength, excellent thermal and electrical conductivity and a high strength-to-weight ratio. Desirable mechanical properties can be achieved by alloying aluminium with other elements like copper, manganese or zinc. For many decades chromate coatings represented the most effective corrosion protection for aluminium alloys. Since their production implies the use of toxic compounds, the use of chromate coatings was banned or restricted in 2002 by European regulations (Restriction of Hazardous Substances (RoHS), Directive 2002/95/EC). In the past decade studies have been directed in searching for new alternatives for chromate coatings which would achieve comparable corrosion protection while being environmentally acceptable. In that context the development of sol-gel coatings is important. Sol-gel is a network of oxides formation of calcium phosphate is formed by the condensation reactions of precursors in a liquid medium. In our laboratory we are devoted to the development of hybrid sol-gel coatings that enable the effective corrosion protection of aluminium and







its alloys (AA2024 and AA7075). The addition of various inhibitors or nano-particles enables the condition of selfhealing properties, i.e., the activation of corrosion protection once the medium conditions, e.g., pH and temperature

We have developed a new hybrid coating for the corrosion protection of metals in various corrosive media. This achievement was awarded as the third best innovation at the University of Ljubljana in 2012. are changed, or the damage at the surface occurs. Hybrid coatings developed in the laboratory were awarded as third best innovation of the University of Ljubljana in 2012. In the field of corrosion protection of aluminium we also collaborate with the Faculty of Technology and Metallurgy University of Belgrade. Vinyltriethoxysilane coatings were investigated using the method of X-ray photoelectron spectroscopy. We proved that the formation of Si–O–Si and Si–O–Al bonding is essential for achieving the good corrosion stability of

We continued with our theoretical investigations of organic corrosion inhibitors, where our principal aim is to better understand how organic corrosion inhibitors act against corrosion at the molecular level and to scrutinize the fundamental principles that govern their corrosion inhibition characteristics. In the past few years we have studied by means of firstprinciple density-functional-theory (DFT) based computer simulations the

interaction of several azole-type corrosion inhibitors with copper surfaces,

while recently the interaction of a few of these molecules with the surfaces

of iron and aluminium have also been investigated. Our findings indicate

that the inhibitor-surface bonding strongly depends on the type of metal and

that the role of metal d-states for the inhibitor-surface bonding is far more

sp-metals the bonding is considerably weaker and inhibitor molecules tend

to chemisorb perpendicularly with unsaturated heteroatom(s) with their

for screening new corrosion inhibitors with potentially superior corrosion

inhibition characteristics, we were able - on the basis of the ascertained

atomic scale details of the inhibitor-surface interactions - to pinpoint some

With respect to the long-term goal of developing more predictive models

 σ -molecular orbitals involved in the molecule-surface bonds.

these coatings. In searching for new alternatives for effective corrosion protection that is environmentally acceptable, we also investigate the use of carboxylic acids. Besides protection, the coatings formed offer other functional properties such as hydrophobicity.



Figure 2: Schematic presentation of a hybrid coating containing a corrosion inhibitor. Such a coating exhibits a self-healing property, i.e., once the coating is damaged, the corrosion inhibitor is activated and heals the coating. Coatings deposited at the metal surface can be painted for additional protection. These coatings are suitable for materials used in the automotive and aerospace industries.

important for transition metals with an open d-band, where the inhibitor molecules can strongly chemisorb parallel to the surface with a pronounced π -d hybridization, while on transition metals with a fully occupied d-band and on

By means of first-principle density-functionaltheory-based computer simulations we have ascertained many details about the interaction of azole corrosion inhibitor molecules with the surfaces of various types of metals, which is now much better understood at the atomic level.

inconsistencies in the usual application of a few electronic parameters that are frequently used in this context and are based on the so-called HSAB (hard and soft acids and bases) concept. A theoretical formalization of the HSAB concept has been derived for molecular systems, yet in the context of corrosion



Figure 3: Electron deformation density of two types of interaction of benzimidazole molecule with metal surfaces. On transition metals with an open d-band the molecule can strongly chemisorb parallel to the surface with a pronounced π -d hybridization (left), whereas on transition metals with a fully occupied d-band and on sp-metals the molecule weakly chemisorbs with unsaturated heteroatom through δ -molecular orbitals (right).

We showed that the CH₃SO + NO₂ reaction can be a source of atmospheric nitrous acid (HONO) emission, that contributes to the production of the hydroxyl radical (OH) leading to a photochemical smog in polluted regions. inhibitors one deals with surfaces that are extended systems. This leads to some ambiguities, which are the source of the above-mentioned inconsistencies. We have shown how these HSAB-based electronic parameters can be consistently applied in the case molecular-surface systems.

Our theoretical investigations of atmospherically relevant radical reactions were based on quantum chemical methods and were continued the examinations of the mechanism of the reaction of the sulphur-containing radicals with NO₂. The methyl sulfinyl radical CH₂SO has been postulated as one of the key and highly reactive intermediates in the atmospheric oxidation of dimethyl sulphide CH3SCH₂ (DMS), which is the largest natural source of reactive sulphur in the troposphere. The mechanism for the CH₂SO + NO₂ singlet radical-radical reaction can be summarized as an initial association of radicals, followed by isomerization and/or the dissociation of intermediates. The direct hydrogen abstraction mechanism is less likely. The results suggest that the CH₂SO + NO₂ reaction is dominated by CH₂S(O)ONO intermediate formation, followed by a dissociation to the CH₂SO₂ + NO products. The CH₂SO₂ dissociation to CH₃ + SO₂ is very likely; however, the final products are CH₃ + SO_2 + NO. The calculation also indicates that the products CH_2SO_2 + HONO and the formation of CH3S(0)NO, are plausible, but their formations would be minor reaction channels.

In the framework of Laboratory for organic and bioorganic chemistry we continued the investigation of the application of the principles of green

chemistry to the transformations of organic compounds. We studied the reactions of the oxidative halogenation of organic compounds in multifunctional ionic liquids and discovered that ionic liquids bearing a nitrate anion represent in the presence of hydrogen bromide or hydrogen chloride an efficient media and reagent for oxidative bromination or chlorination of aromatic molecules. The combination of ethylammonium nitrate (EAN) or propylammonium nitrate (PAN) with aqueous HBr or HCl was used for the efficient and selective halogenation of activated or partly deactivated aromatic molecules. An ionic liquid could be regenerated and efficiently reused at least five times. Ionic liquids from the group of metly-butyl-imidazolium salts (BMIM) bearing sulfonic group on the cationic part of the molecule and nitrate anion [BMIM(SO₂H)][NO₂], in the presence of HBr or HCl also exhibited efficient and selective reactivity for the halogenation of aromatic compounds. The methodology was considerably improved by the preparation of ionic liquids bearing both nitrate and halogenide anions [BMIM(SO₂H)] $[(NO_2)_{(X)_2}]$ and an x:y ratio equal to 1 was established as the best choice. We further studied the halogenation of aromatic molecules and arvl-alkyl ketones with N-halosuccinimides (NXS) in ionic liquids and established that the acidic functionality in the cationic backbone of ionic liquid considerably



Figure 4: A schematic view: Dimethyl sulphide, CH3SCH3, as a source of atmospheric nitric acid, HONO.

We discovered and developed a new method for the oxidative halogenation of organic compounds using interhalogen iodine(I) compounds.

accelerates the halogenation process. A variety of aromatic compounds and aryl-alkyl ketones were thus halogenated with a combination of [BMIM(SO,H)][OTf] and NXS (X = Br, Cl, I) and the ionic liquid could be regenerated and reused at least ten times. We studied the chemistry of polyvalent iodine(I) compounds and developed a new

method for their preparation using molecular iodine, hydrogene peroxide as the oxidant and HCl as the activator of the process. These compounds were isolated as tetraelkyl or pyrindium salts, which were further used as an iodinating reagent for organic compounds. This method represents an original, new approach where iodo(I) species play the role of the source of the iodine atoms. The presence of hydrogen chloride is essential, but only in the presence of catalytic amounts, which makes this method very attractive.

We discovered and developed the new synthetic method for the transformation of ketones and aldehydes into dihydroperoxides, important precursors in the synthesis of bioactive peroxides. The advantage of this method is that no catalyst was needed for the efficient process using 30% aqueous hydrogen peroxide as the oxidant.

In the framework of the Centre of Excellence CIPKeBiP and the collaboration of the high-tech company ACIS BIO we have collaborated in the directed synthesis of potential bioactive compounds from the family of pantetinic acid and derivatives of malonic acid as precursors in polyketide biosynthesis. We have collaborated with the company Semenarna on the synthesis of gamethocidic active compounds used in processes for the production of plant hybrids.

Some outstanding publications in the past year

- 1. Milošev, I.: The effect of biomolecules on the behaviour on CoCrMo alloy in various simulated physiological solutions, Electrochim. Acta, 2012, 78, pp. 259-273
- Milošev, I., Jovanović, Ž., Bajat, J.R., Jančić-Heinemann, R., Mišković-Stanković, V. B.: Surface analysis and 2. electrochemical behaviour of aluminium pretreated by vinyltriethoxysilane films in mild NaCl solution, J. Electrochem. Soc., 2012,1 59, pp. C303-C311
- 3. Kovačević, N., Kokalj, A.: Chemistry of the interaction between azole type corrosion inhibitor molecules and metal surfaces, Mater. Chem. Phys., 2012, 137, pp. 331-339
- Lesar, A.: Product channels in the reaction of the CH₂SO radical with NO₂: DFT and ab initio studies, Int. J. 4. Quantum Chem., 2012, 112, pp. 1904–1912
- 5. Bedrač, L., Iskra, J.: Dihaloiodates(I): synthesis with hydrogen peroxide and their halogenating activity, Tetrahedron Lett., 2012, 53, pp. 5555-5558

Awards and appointments

- Anton Kokalj: Pregl Awards for Exceptional Achievements for Important Scientific Contribution in the Field 1. of Chemistry and Associated Science, Ljubljana Slovenia, 2012
- 2. Peter Rodič, Ingrid Milošev, Jernej Iskra, Barbara Kapun: Rector's Award for the third best innovation of University in Ljubljana, for the year 2012



Figure 5: Oxidative halogenation of organic compounds using interhalogene iodine(I) compounds.

INTERNATIONAL PROJETCS

- 1. Testing CIs for metals in different media, with emphasis on acidic media and methane sulfonic acid (MSA)
 - BASF SE
- Dr. Matjaž Finšgar
 Reactions of S-containing radicals with amines and NO_x: A theoretical study Slovenian Research Agency
- Dr. Antonija Lesar
- Atomistic computer simulations of N₂O dissociation on Rh(100) and Rh(110) surfaces and the role of coadsorbed oxygen Slovenian Research Agency
- Dr. Anton Kokalj 4. Transformations of organic compounds under green reaction conditions Slovenian Research Agency
- Prof. Stojan Stavber5. Improvement of functionality of biomedical and engineering materials Slovenian Research AgencyProf. Ingrid Milošev

RESEARCH PROGRAMS

- 1. Multiphase nanoarchitectures: development, physical-chemical characterization and simulation of processes
- Prof. Ingrid Milošev 2. Bioanorganic and bioorganic chemistry
- 2. Bioanorganic and bioorganic chemistry Prof. Stojan Stavber

VISITORS FROM ABROAD

- Dr. Stefano Fabris, IOM-CNR DEMOCRITOS and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, 7. 2. 2012
- 2. Dr. Robert Vianello, Ruđer Bošković Institute, Zagreb, Croatia, 29. 2. 2012

STAFF

Researchers

- 1. Asst. Prof. Jernej Iskra
- 2. Dr. Anton Kokalj
- 3. Dr. Antonija Lesar
- 4. Prof. Ingrid Milošev, Head
- 5. Prof. Stojan Stavber
- Postdoctorial associates
- Dr. Matjaž Finšgar, left 01.07.12
 Dr. Sebastijan Peljhan, left 01.06.12
- Postgraduates
- 8. Leon Bedrač, B. Sc.

BIBLIOGRAPHY

ORIGINAL SCIENTIFIC ARTICLE

- 1. Leon Bedrač, Jernej Iskra, "Dihaloiodates(I): synthesis with hydrogen peroxide and their halogenating activity", *Tetrahedron lett.*, vol. 53, no. 41, pp. 5555-5558, 2012.
- Anton Kokalj, "On the HSAB based estimate of charge transfer between adsorbates and metal surfaces", *Chem. phys.*, vol. 393, issue 1, pp. 1-12, 2012.
- 3. Nataša Kovačević, Anton Kokalj, "Chemistry of the interaction between azole type corrosion inhibitor molecules and metal surfaces", *Mater. chem. phys.*, vol. 137, no. 1, pp. 331-339, 2012.
- Nataša Kovačević, Boris Pihlar, Vid Simon Šelih, Ingrid Milošev, "The effect of pH value of a simulated physiological solution on the corrosion resistance of orthopaedic alloys", *Acta chim. slov.*, vol. 59, no. 1, pp. 144-155, 2012.

- R & D GRANTS AND CONTRACTS
- Role of molecular structure of inhibitors and their selfassembling in corrosion protection of metal surfaces Dr. Anton Kokalj
- The effect of bio-environment on the stability of biomedical metallic materials Prof. Ingrid Milošev
- Modifications of surface of metallic biomaterials and their interaction with bioenvironment Prof. Ingrid Milošev
- Use of green energy sources: New functional nanomaterials on the base of polyzometalates and TiO2 nanostrucutres for production of hydrogen by catalytic oxidation of water – NANOleaf Asst. Prof. Jernej Iskra
- SURFUNCTI: Controlled surface structuring and surface functionalisation of advanced biomedical titanium alloys for ortopaedic implants Prof. Ingrid Milošev

NEW CONTRACTS

- Alternative synthesis of pharmaceutical compounds Krka, d. d., Novo mesto Asst. Prof. Jernej Iskra
- Consulting on the area of organic chemistry stressing the syntesis of organic compounds
 Low Proceeding of the syntesis of organic chemistry stressing the syntesis of organic compounds
- ACIES BIO, d. o. o. Prof. Stojan Stavber
- Ecology laboratory with mobile unit Ministrstry of Defence Asst. Prof. Jernej Iskra
- Ianina Santana, INTEMA, Division of Electrochemistry and Corrosion, Universidada Nacional de Mar del Plata, Argentina, 16. 9–16. 10. 2012
- Prof. Cristiano Zonta, University of Padova, Italy, 23.–24. 10. 2012
- 9. Simona Jerenec, B. Sc.
- 10. Nataša Kovačević, B. Sc.
- 11. Jerca Pahor, B. Sc.
- 12. Rok Prebil, B. Sc.
- 13. Peter Rodič, B. Sc.
- Katarina Starkl, B. Sc.
 Dejan Vražič, B. Sc.
- 16. Gregor Žerjav, B. Sc.
- Technical officers
- 17. Barbara Kapun, B. Sc.
 - 5. Antonija Lesar, "Product channels in the reaction of the CH_3SO radical with NO_2 : DFT and ab initio studies", *Int. j. quant. chem.*, vol. 112, no. 8, pp. 1904-1912, 2012.
 - 6. Tatsuo Matsushima, Anton Kokalj, Hideo Orita, Toshitaka Kubo, Masataka Sakurai, Takahiro Kondo, Junji Nakamura, "N₂ emissionchannel change in NO reduction over stepped Pd(211) by angleresolved desorption", *Surf. sci.*, vol. 606, no. 13/14, pp. 1029-1036, 2012.
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 - 8. Ingrid Milošev, "The effect of biomolecules on the behaviour of CoCrMo alloy in various simulated physiological solutions", *Electrochim. acta*, vol. 78, pp. 259-273, 2012.

- Ingrid Milošev, Ž. Jovanović, Jelena B. Bajat, R. M. Jančić-Heinemann, Vesna B. Mišković-Stanković, "Surface analysis and electrochemical behavior of aluminum pretreated by vinyltriethoxysilane films in mild NaCl solution", *J. Electrochem. Soc.*, vol. 159, no. 7, pp. C303-C311, 2012.
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- 11. Ingrid Milošev, Barbara Kapun, "The corrosion resistance of Nitinol alloy in simulated physiological solutions. Part 2, The effect of surface treatment", *Mater. sci. eng., C, Biomim. mater., sens. syst.*, vol. 32, no. 5, pp. 1068-1077, 2012.
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- 13. Ingrid Milošev, Mirjana Metikoš-Huković, Željka Petrović, "Influence of preparation methods on the properties of self-assembled films of octadecylphosphonate on Nitinol: XPS and EIS studies", *Mater. sci. eng., C, Biomim. mater., sens. syst.*, vol. 32, no. 8, pp. 2604-2616, 2012.
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- 16. Zoi Salta, Agnie Mylona Kosmas, Antonija Lesar, "Computational investigation of the peroxy radicals CH3S(0)nO0 and the peroxynitrates CH3S(0)nO0N02 (n = 0, 1, 2)", *Computational and theoretical chemistry*, vol. 1001, pp. 67-76, 2012.
- 17. Primož Titan, Vladimir Meglič, Jernej Iskra, "Combining ability and heterosis effect in hexaploid wheat group", *Genetika (Beogr.)*, (Acta biologica Iugoslavica), vol. 44, no. 3, pp. 595-609, 2012.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- Leon Bedrač, Jernej Iskra, "Dihalojodati(I): z vodikovim peroksidom in njihova raktivnost: synthesis with hydrogen peroxide and their reactivity", In: *Slovenski kemijski dnevi 2012, Portorož, 12.-14. september 2012*, Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2012, 11 pp.
- 2. Jerca Pahor, Gaj Stavber, Stojan Stavber, "Aerobno oksidativno jodiranje organskih spojin, katalizirano z dušikovo(V) kislino", In: *Slovenski kemijski dnevi 2012, Portorož, 12.-14. september 2012,*

Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2012, 11 pp.

- Kelly Peeters, Jernej Iskra, Tea Zuliani, Janez Ščančar, Radmila Milačič, "Synthesis of ¹¹⁷Sn enriched tributyltin", In: *Slovenski kemijski dnevi* 2012, Portorož, 12.-14. september 2012, Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2012, 11 pp.
- 4. Ajda Podgoršek, Jernej Iskra, Stojan Stavber, Margarida F. Costa Gomes, Agílio A. H. Pádua, "Kemija v alternativnem reakcijskem mediju: vpliv strukturnih in energijskih aspektov solvatacije: effect of structural and energetic aspects of solvation", In: *Slovenski kemijski dnevi 2012, Portorož, 12.-14. september 2012,* Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2012, 11 pp.
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INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

- 1. Jernej Iskra, "Green methods in halogenation of heterocycles", In: *Halogenated heterocycles: synthesis, application and environment,* (Topics in heterocyclic chemistry, 27), Alicia Decker, Jernej Iskra, ed., Heidelberg [etc.], Springer, 2012, pp. 269-308.
- Ingrid Milošev, "CoCrMo alloy for biomedical applications", In: Biomedical applications, (Modern aspects of electrochemistry, 55), Stojan S. Djokić, ed., New York [etc.], Springer, cop. 2012, pp. 1-72.

PATENT APPLICATION

1. Primož Titan, Jernej Iskra, Vladimir Meglič, *Chemical hybridization of hermaphrodite plant species with easily soluble derivatives of oxanilic acid*, P-201200130, Urad RS za intelektualno lastnino, 24.4.2012.

MENTORING

- 1. Simon Kovač, The effect of various bearings of total hip prostheses (metal-on-polyethylene and metal-on-metal) on the mid-term results of clinical and radiological analysis: doctoral dissertation, Ljubljana, 2012 (mentor Vinko Pavlovčič; co-mentor Ingrid Milošev).
- 2. Sebastijan Peljhan, *Simulations of corrosion inhibition mechanisms of benzotriazole as copper corrosion inhibitor in chloride media:* doctoral dissertation, Ljubljana, 2012 (mentor Anton Kokalj).

ELECTRONIC CERAMICS DEPARTMENT

K-5

The Electronic Ceramics Department is active in the research of the synthesis, properties and applications of materials for electronics and energetics, mainly complex multifunctional materials and structures. The materials of interest include ceramic piezoelectrics, ferroelectrics, relaxors, multiferroics and conductive oxides. The emphasis is on the development of properties by synthesis and structure on the nano-, micro- and macro-levels. The group also works on the principles of basic technologies of ceramic pressure sensors, ceramic micro-electromechanical systems (MEMS) and flexible electronics.

Within the research on environment-friendly lead-free piezoelectric ceramics based on alkaline niobates we studied the influence of the different Nb₂O₅ polymorphs, i. e., the orthorhombic and monoclinic Nb₂O₅ modifications, on the solid-state synthesis of the K_{0.5}NbO₃ (KNN) solid solution. Two batches of KNN were prepared from the respective Nb₂O₂ polymorphs, both of which were pre-milled and subsequently mixed with the alkali carbonates. X-ray diffraction and transmission electron microscopy analyses showed that the as-milled monoclinic Nb₂O₂ Head: consisted of large monoclinic particles together with orthorhombic nanocrystals. The mixed-phase Nb₂O₅ reacted **Prof. Marija Kosec**

with the carbonates to form the K_vNa_vNbO_a solid solutions with varying K/Na molar ratios. In contrast, the crystal structure of the orthorhombic Nb₂O₅ was not modified by the milling process. It reacted with the carbonates to form a homogeneous solid solution. The study confirmed a significant influence of the Nb₂O₅ crystal structure on the homogeneity of the KNN and, consequently, on its densification.

We developed a simple and efficient "top-down" approach for the preparation of NaNbO₂ nanopowders. We prepared the submicron-sized NaNbO₂ powder by solid-state synthesis, and subsequently milled it in an agitator bead mill. The milling process was optimized to yield nanoparticles with an average size of ~25 nm, which is comparable to the particle sizes obtained by solution-based chemical routes or mechanochemical synthesis. The nanopowder exhibited a better compaction behaviour, resulting in powder compacts with an about six times lower average pore radius and a narrower pore size distribution, in comparison with the submicron-sized powder. The powder will be further used for studying the sintering behaviour of NaNbO₂.

In collaboration with the Institute of Physics of Academy of Sciences of the Czech Republic from Prague, we evaluated for the first time the lattice dynamics of KTaO₂ ceramics. Using infrared spectroscopy analysis, we identified three polar modes characteristic for perovskites with the cubic structure. The lowest-frequency TO1 mode (soft mode) strongly softens on cooling.

Prof. Marija Kosec, the long-term Head of the Electronic Ceramics Department, died on 23 December 2012. Prof. Kosec was the Ambassador of Science of the Republic of Slovenia (2003), winner of the Zois award for outstanding scientific and development achievements in the field of ceramic materials (2006) and the Puh recognition award for development achievements (2009). She was also one of the rare European female scientists who received a distinguished award "Ferrroelectrics Recognition Award, IEEE Ultrasonics, Ferroelectrics and Frequency Control Society" for her exceptional contribution to the science and processing technology of ferroelectric powders, bulk ceramics, thin and thick films.

The dielectric permittivity, measured in the kHz and GHz frequency range, is mainly attributed to the intrinsic polar lattice modes' contribution. Unlike in other ferroelectric or incipient ferroelectric perovskite ceramics, the soft-mode frequency agrees with the values measured in KTaO, single crystals, suggesting a negligible influence of the grain boundaries on the dielectric response of the KTaO, ceramics.

Within the activities on lead-based piezoelectric ceramics, we focused on the solid-state synthesis and characterization of the Pb(Zr,Ti)O₂ (PZT) and tetragonal stabilized zirconia (TZ) composites. A possible way to toughen the originally brittle PZT ceramics is by introducing zirconia particles. Within the EU 7FP project HIPERact and in collaboration with the Technische Universität Darmstadt, we found that the addition of TZ leads to transformation toughening and reduces the ferroelastic toughening of the PZT ceramics. In order to separate the two toughening mechanisms, we studied the cubic lanthanum-modified PZT (PLZT) with and without TZ additions. A rising R-curve behaviour, which was experimentally observed in the PLZT-TZ composites, suggested phase-transformation toughening. This confirmed that the TZ addition indeed leads to a partial phase *composition and temperature*.



Figure 1: (a) Tetragonal (open symbols) and rhombohedral (filled symbols) spontaneous lattice distortions and (b) coercive stress of soft PZT, measured at the Technische Universität Darmstadt, as a function of





Figure 2: (a) Relative piezoelectric coefficient d_{33} of BiFeO₃ ceramics as a function of amplitude and frequency of stress, measured at Ecole Polytechnique Federale de Lausanne, Switzerland. The increase in the d_{33} with the stress amplitude suggests a contribution from 71° and 109° domain walls. (b) Identification of 71° and 109° domains in BiFeO₃ ceramics by means of selected area electron diffraction. Figures b1 and b3 show the experimental diffraction patterns with typical spot splitting, which are in agreement with the simulated patterns for b2) 109° and b4) 71° domains.

transformation toughening of PZT. In addition to the studies on composites, we performed an X-ray diffraction analysis combined with the Rietveld refinement method to analyse the phase composition of PZT with different Zr/Ti molar ratios and as a function of temperature. The Rietveld refinement method was used to determine the unit-cell parameters and the corresponding tetragonal and rhombohedral lattice distortions. The obtained lattice distortions were compared with the measured stress-strain curves of the PZT samples. The compositions rich in Ti showed an increased ferroelastic coercive stress, which we attribute to the larger tetragonal distortion (Figure 1).

Within the 7FP EU project CERAMPOL and in collaboration with the research partner HIPOT-RR we studied the integration of **PZT-based piezoelectric actuators** in **waste-water cleaning systems**.

We continued our studies on the piezoelectric properties of **multiferroic BiFeO**₃. In collaboration with the Ecole Polytechnique Federale de Lausanne, Switzerland, we studied systematically the dependence of the piezoelectric d_{33} coefficient on the frequency and amplitude of the applied stress field. The response of the ferrite is strongly nonlinear, which means that the d_{33} depends upon the stress amplitude (Figure 2a). The nonlinearity suggests an irreversible, non-180°, domain-wall contribution to the piezoelectric response. This relative contribution is comparable to the contribution measured in PZT, which gives BiFeO₃ and BiFeO₃-based compositions a great potential for piezoelectric applications. Using transmission electron microscopy we also performed a study of the domain structure of the ferrite. In addition to the defects, a characteristic of octahedrally tilted structures, i.e., the antiphase boundaries, we also identified the 71° and 109° domain walls by means of selected-area electron diffraction (Figure 2b).

In the frame of the research on **lead-free ferroelectric and relaxor thin films** prepared via solution synthesis, we collaborated with the University of Nova Gorica and the Faculty of Mathematics and Physics, University of Ljubljana. We investigated the local ordering of niobium and tantalum in the $\text{KTa}_{0.6}\text{Nb}_{0.4}\text{O}_3$ sols after different reflux times, ranging from 1 to 48 hours. In fact, within an earlier study, we found that the reflux strongly influenced the crystallization of the perovskite phase during the annealing of the films. By varying the reflux time, the Ta

environment did not change; however, in the case of Nb, a stable state was achieved after only 24 hours of reflux.

The aim of the **transparent electronics** is to create transparent or translucent elements, e.g., thin-film transistors. The active layers, composed typically of dielectric, conductive or semiconductive materials, are deposited onto glass or polymer substrates, which can be annealed only at relatively low temperatures. Using solution synthesis we prepared high-K dielectric thin films based on Ta_2O_5 -Al_2O_3-SiO_2 with the atomic ratio Ta: Al : Si = 8: 1 : 1 on glass substrates. After annealing at 300°C and 400°C, the measured dielectric permittivity at 100 kHz was 18 and 22, respectively; in both cases, the dielectric loss factor tand was 0.03. The leakage current density was lower in the films prepared at 300°C. The Ta_2O_5 -Al_2O_3-SiO_2 films exhibited a lower leakage current density than the Ta_2O_5 films, prepared at the same temperature, which means that they could be suitable for integration into semiconductor elements. Within the frame of p-type semiconductors we studied the solid-state synthesis of CuAlO₂. The inert atmosphere was found to be crucial for the preparation of phase-pure CuAlO₂. The research took place in the frame of the 7 FP EU project ORAMA.

We continued the research on the processing of PZT-based piezoelectric thick films using the electrophoretic deposition process (EPD) for high-frequency, ultrasound, transducer applications. We systematically studied the

Prof. Marija Kosec was the president of the 48th MIDEM conference on microelectronics, elements and materials with the Workshop on Ceramic Microsystems, which was held on 19–21 September 2012 at Otočec, Slovenia. She managed to attract a large number of representatives from Slovenian industry and, thus, crucially contributed to the success of the conference. thickness and the microstructure of PZT thick films as a function of the properties of the suspension, the deposition and the sintering conditions. In collaboration with the University Francois-Rabelais from Tours, France, we integrated a homogeneous PZT thick film deposited on a curved substrate, with a thickness of $30 \,\mu\text{m}$, a density of $85 \,\%$ and a thickness-coupling factor of $50 \,\%$, into a real-time ultrasonic probe (Figure 3). The transducer operates at 40 MHz and enables *in vivo*, non-destructive high-resolution imaging of biological tissues for medical investigations and diagnostics.

We optimized the screen-printing conditions for the deposition of $K_{0.5}Na_{0.5}NbO_3$ (KNN) thick films. The measurements of the piezoelectric properties of the resulting thick films revealed that the relative reduction of

the piezoelectric d_{33} coefficient of KNN due to the substrate clamping is smaller in comparison with the reduction in lead-based perovskites, such as PZT. This gives the KNN thick films an advantage over the lead-based films.

In collaboration with the Instituto de Ciencia de Materiales de Madrid, Spain, we studied the domain structure of $Pb(Mg_{1/3}Nb_{2/3})O_3$ -PbTiO₃ (PMN-PT) thick films by piezoresponse force microscopy. The thick films were prepared by the screen-printing method and subsequent firing. Complex, non-180°, domain configurations with strong variations in the characteristic length (from micro- to the nano-scale) were found. (Figure 4) In addition,

the mobility of the domain walls under an electric field was demonstrated, which is the key to the relatively high electromechanical response of the PMN-PT films.

We studied the **electrocaloric (EC) effect** in PMN-PT ceramics and thick films. In addition to the large electrostrictive response, already reported in 0.65PMN-0.35PT/Pt self-standing thick films, the existence of a large EC effect of a similar magnitude as found in bulk ceramics was also experimentally confirmed in thick films.

Within the 7 FP EU project Microflex we studied the integration of piezoelectric elements on temperature-sensitive textile substrates. The active material was deposited either by screen-printing or ink-jet printing with subsequent curing by ultraviolet light or by heating at a maximum temperature of 150°C. We succeeded to develop the temperature and strain sensor on polycotton and inflammable polyamide (Figure 5).

We continued the investigations on LTCC (Low-Temperature Co-fired Ceramics) materials used for 3D structures for different electromechanical (MEMS - Micro Electro Mechanical Systems) and chemical microsystems. Within the collaboration with the Montanuniversität Leoben, Austria, the influence of the firing conditions on the microstructural and mechanical

a) 100 µm PZT Au PZT substrate c) Vessel Tendon C) Vessel Tendon

Figure 3: $Pb(Zr,Ti)O_3(PZT)$ thick film on a porous PZT substrate, b) photograph of the ultrasound transducer prototype, which was integrated into a probe (collaboration with the University Francois-Rabelais from Tours, France), c) image of the normal skin of a forearm taken at the University Francois-Rabelais.

characteristics of Du Pont LTCC materials was investigated. After firing at 800°C the porosity of the LTCC was 7%, the modulus of elasticity was 100 GPa and the mechanical strength was 140 MPa. After firing at 875°C the porosity decreased to 1%, while the modulus of elasticity and the mechanical strength increased to 120 GPa and 300 MPa, respectively. At higher firing temperatures, up to 1000°C, the characteristics remained almost unchanged. This result suggests that the tested LTCC material can be fired within a wide temperature range, and it still preserves mechanical characteristics, suitable for the production of MEMS and micro-systems.

Within the programme JE PECS of the European Space Agency (ESA) and the project CERACON, which is about the **production of LTCC micro-reactors** and the necessary periphery for catalytic transformation of methanol and water into hydrogen for low-temperature fuel cells, we successfully designed and realised LTCC structures with large buried cavities (with a volume of 3 cm³).

Together with the research partner HIPOT-RR we further acquired new knowledge in the field of materials, design and construction of **ceramic pressure sensors based on LTCC technology**. The results enabled (i) a significant

decrease of the temperature dependence of the sensors' characteristics, (ii) the production of ceramic pressure sensors with long-term stability and (iii) miniaturisation. As an example, we emphasize the developed ceramic pressure sensor for the 0-34 bars pressure range and with dimensions of 5.9 mm x 5.9 mm (together with contacts 7.2 mm) x 0.75 mm. The acquired "know-how" allowed the industrial partner HYB d.o.o to develop new pressure sensors based on the LTCC technology. Temperature-dependent thick film resistors (thermistors) were integrated on LTCC structures as well. This enabled the development of sensors that combine pressure- and temperature-sensing elements. A part of the investigations was undertaken within the EUREKA project, which ended successfully this year. With the research partner HIPOPT-RR and with the colleagues from the Technical University Brno, Czech Republic, we performed an extensive study of the influences of thick-film conductors on the noise indices of the thick-film resistors on alumina and LTCC substrates. The results indicated a lower noise for the resistor terminated with silver base conductors.

In cooperation with the company **ETI d.d. Izlake** we investigated materials based on steatite and cordierite. In the case of the steatite, we studied the influence of the type of the raw materials, the milling conditions and the sintering temperature on the microstructure and properties of the ceramics. We fabricated a new type of alkali-free dense steatite with a homogeneous microstructure, high specific resistivity, low dielectric constant and low



Figure 4: PFM images of the $Pb(Mg_{1/3}Nb_{2/3})O_3$ - $PbTiO_3(PMN-PT)$ thick-film surface; a) topography, b) in-plane amplitude image and c) in-plane phase image. d) Possible schematic representation of polarization, assuming the three domains inside the largest twin to be 180° for simplicity (in collaboration with Instituto de Ciencia de Materiales de Madrid, Spain).



Figure 5: Stretchable strain-gauge fabric with the controlling LED developed within the 7FP EU project Microflex. At 1.5% of expansion strain the resistivity increases from the kOhm to the MOhm range.

loss factor, planned as the base and housing of the fuses. We improved the reproducibility of the porous cordierite in the high-scale production through the control of the composition and morphology of raw materials, and the modification of the milling procedure. The resulting cordierite with a high thermal shock resistance and a high flexural strength was used for processing of the elements for insulation.

Some outstanding publications in the past year

- Uršič, H., Ricote, J., Amorin, H., Holc, J., Kosec, M., Alguero, M.: Ferroelectric domain configurations in 0.65Pb(Mg_{1/3}Nb_{2/3})O₃-0.35PbTiO₃ thick films determined by piezoresponse force microscopy. J. Phys. D: Appl. Phys. 45, 2012, 265402, p. 11
- Kupec, A., Malič, B., Tellier, J., Tchernychova, E., Glinšek, S., Kosec, M.: Lead-free ferroelectric potassium sodium niobate thin films from solution: composition and structure. J. Am. Ceram. Soc. 95 [2], 2012, pp. 515-523
- Kuščer, D., Levassort, F., Lethiecq, M., Abellard, A.-P., Kosec, M.: Lead-zirconate-titanate thick films by electrophoretic deposition for high-frequency ultrasound transducers, J. Am. Ceram. Soc., 95 [3], 2012, pp. 892-900
- Rojac, T., Bencan, A., Drazic, G., Kosec, M., Damjanovic, D.: Piezoelectric nonlinearity and frequency dispersion of the direct piezoelectric response of BiFeO₃ ceramics. J. Appl. Phys., 112, 2012, 064114

Awards and appointments

1. Best Poster Paper Award at TCM 2012 for Raluca Camelia Frunza, Crete, Greece, 26. 11. 2012

Patents granted

- Luca Gregoratti, Marco Peloi, Marija Kosec, Danjela Kuščer, A material in the form of lithium fluoride powder containing colour centres, method for preparation and use thereof, IT1397095, Notarbartolo & Gervasi S.P.A., 28.12.2012.
- Janez Holc, Kostja Makarovič, Darko Belavič, Marko Hrovat, Marija Kosec, Boris Jordan, The manufacturing process of voids in the ceramic multi layered structures, SI23761 (A), Urad RS za intelektualno lastnino, 31.12.2012.
- 3. Helena Razpotnik, Ivan Lavrač, Janez Holc, Danjela Kuščer, Marija Kosec, Procedure for fabrication of alumina porcelain with improved mechanical properties, SI23546 (A), Urad RS za intelektualno lastnino, 31.5.2012.

INTERNATIONAL PROJECTS

- 1. 7. FP HIPER-Act: Novel technology for high-performance piezoelectric actuators European Commission
- Prof. Marija Kosec, Asst. Prof. Andreja Benčan Golob 2. 7. FP - MICROFLEX: Micro fabrication production technology for MEMS on new
- emerging smart textiles/flexibles European Commission
- Prof. Marija Kosec, Dr. Janez Holc, Prof. Tomaž Kosmač
- 3. 7. FP ORAMA: Oxide materials towards a matured post-silicon electronics era European Commission
- Prof. Marija Kosec, Asst. Prof. Barbara Malič
 4. 7. FP CERAMPOL: Ceramic and polymeric membrane for water purification of heavy metal and hazardous organic compound European Commission
- Asst. Prof. Danjela Kuščer Hrovatin, Dr. Tadej Rojac
- 7. FP PI: The Piezo Institute European expertise centre for multifunctiona and integrated piezoelectric devices European Commission
- Prof. Marija Kosec
- CERACON: Integration and control of liquid fuel processor based on ceramic microsystems ESA/ESTEC
- Asst. Prof. Marko Hrovat, Dr. Gregor Dolanc
- COST MP0904, SIMUFER: Single- and multiphase ferroics and multiferroics with restricted geometries

COST Office Prof. Barbara Malič

- FERRO-PATCH: Frequency and polarisation agile microstrip patch antenna based on ferrelectric varactors
 - ESA/ESTEC Prof. Barbara Malič
- Studies of the processing influence on functional properties of ferroelectric materials for microwave applications
 Studies Descent Access
- Slovenian Research Agency Prof. Marija Kosec
- Low temperature processing of functional oxide thin films
- Slovenian Research Agency Prof. Barbara Malič
- Solution processing of thin films for transparent electronics (TRANS) Slovenian Research Agency Prof. Marija Kosec
- Dielectric spectroscopy and tunability of low-temperature processed complex perovskites
- Slovenian Research Agency Prof. Marija Kosec

RESEARCH PROGRAM

1. Electronic ceramics, nano-, 2D and 3D structures Prof. Marija Kosec

R & D GRANTS AND CONTRACTS

- Textured ceramic films for sensors and actuators Prof. Marija Kosec
- 2. Oxide-based components for transparent electronics Prof. Barbara Malič
- Ceramic materials for 3D structures and study of functional properties 3. Dr. Janez Holc
- 4. Materials and technologies for chemical microsystems Asst. Prof. Andreja Benčan Golob
- Pb(Sc0.5Nb0.5)O3-PbTiO3 thick films for sensor and actuator applications Dr. Hana Uršič Nemevšek
- 6 IPCTECH: New generation of 3D integrated passive components and microsystems in LTCC technology

Asst. Prof. Marko Hrovat

VISITORS FROM ABROAD

- 1. Andre-Pierre Abellard, Université François Rabelais, Tours, France, 23. 1.-1. 2. 2012
- Nataša Samardžić, Faculty of Technical Sciences, Novi Sad, Serbia, 30. 1.-7. 2. 2012
- Dandan Wei, School of Electronic and Information Engineering, Xi´an Jiaotong 3.
- University, Xi´an, China, 1. 3.-30. 5. 2012 Gaoqun Zhang, School of Electronic and Information Engineering, Xi´an Jiaotong 4.
- University, Xi ´an, China, 1. 3.-30. 5. 2012 Dr. Carmen Galassi, Institute of Science and Technology for Ceramics, National 5.
- Research Council, Faenza, Italy, 28.-30. 3. 2012 Prof. Biljana Stojanović, Institute of Multidisciplinary Research, University of Belgrade, 6.
- Belgrade, Serbia, 2. 4.-4. 6. 2012 Prof. Christos Likos, Faculty of Theoretical Physics, Universität Wien, Vienna, Austria, 7.
- 5-6 4 2012 Prof. Andreas Klein, Technische Universität Darmstadt, Darmstadt, Germany, 8. 4.-14.4.2012
- Dr. Jan Petzelt, Institute of Physics, Academy of Sciences, Prague, Czech Republic, 24 - 26 4 2012
- 10. Candice Thomas, Grenoble Institute of Technology, Grenoble, France, 21. 5.-27. 7. 2012

STAFF

Researchers

- Asst. Prof. Andreja Benčan Golob 1.
- Dr. Elena Chernyshova'
- Dr. Janez Holc, retired 30.06.12 3.
- Asst. Prof. Marko Hrovat 4.
- Prof. Marija Kosec, Head, died 23.12.12 5.
- Asst. Prof. Danjela Kuščer Hrovatin 6.
- Prof. Barbara Malič
- Dr. Tadej Rojac 8

Dr Marina Santo Zarnik 0

- Postdoctorial associates
- 10. Dr. Sebastjan Glinšek, on postdoctoral leave since 01.09.12
- 11. Dr. Gregor Trefalt, on postdoctoral leave since 01.06.12
- 12. Dr. Hana Uršič Nemevšek
- 13. Dr. Katarina Vojisavljević

Postgraduates

- 14. Tina Bakarič, B. Sc. 15. Raluca-Camelia Frunza, B. Sc.
- 16. Jitka Hreščak, B. Sc.
- 17. Evgeniya Khomyakova, B. Sc.

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ORIGINAL SCIENTIFIC ARTICLE

- 1. Darko Belavič, Marko Hrovat, Gregor Dolanc, Marina Santo-Zarnik, Janez Holc, Kostja Makarovič, "Design of LTCC-based ceramic structure for chemical microreactor", Radioengineering (Prague), vol. 21, issue 1, pp. 195-200, 2012.
- 2. Andreja Benčan, Barbara Malič, Silvo Drnovšek, Jenny Tellier, Tadej Rojac, Jernej Pavlič, Marija Kosec, Kyle Webber, Jürgen Rödel, Dragan Damjanović, "Structure and the electrical properties of Pb(Zr, Ti)O3-

NEW CONTRACTS

- Development of high-temperature fuel cells with methanol reformer on a silicon wafer 1 University of Ljubljana Dr. Hana Uršič Nemevšek
- 2. Investigation of steatite materials types C220, C221 and C230 Razvojni center eNeM Novi Materiali, d. o. o.
- Asst. Prof. Danjela Kuščer Hrovatin 3. Research in the field of cordierite materials type C410, C520, C530 Razvojni center eNeM Novi Materiali, d. o. o. Prof. Marija Kosec
- 11. Dr. Kyle Webber, Technische Universität Darmstadt, Materials Science Department, Nichtmetallisch Anorganische Werkstoffe (NAW), Darmstadt, Germany, 23.–25. 5. 2012
- 12. Prof. Mamoru Senna, Keio University, Yokohama, Japan, 5.–10. 6. 2012
- Julian Walker, School of Materials, Science and Engineering, University of New South 13. Wales, Sydney, Australia, 16. 7.-19. 10. 2012, 15. 12. 2012
- 14. Dr. Phillipe Thomas, SPCTS, European Ceramics Centre, Limoges, France, 25. 7. 2012
- 15. Dr. Cristina Ciomaga, Faculty of Physics, University Al. J. Cuza of Iasi, Iasi, Romania, 16.-23. 9. 2012
- 16. Nadejda Horchidan, Faculty of Physics, University Al. J. Cuza of Iasi, Iasi, Romania, 1.-22. 10. 2012
- 17. Prof. Raul Bermejo, Institute of Structural and Functional Ceramics, Montanuniversität Leoben, Leoben, Austria, 18. 9. 2012
- 18. Dr. Jenny Jouin, SPCTS, European Ceramics Centre, Limoges, France, 8.-13. 10. 2012 Dr. Oana Catalina Mocioiu, Institute of Physical Chemistry Ilie Murgulescu, Bucharest, 19. Romania 12-25 11 2012
- Hermine Stroescu, Institute of Physical Chemistry Ilie Murgulescu, Bucharest, Romania, 20 12.-25. 11. 2012
- 18. Jurij Koruza, B. Sc.
- 19. Alia Kupec, B. Sc.
- 20. Kostja Makarovič, B. Sc.
- 21. Oleksandr Noshchenko, B. Sc.
- 22. Jernej Pavlič, B. Sc. 23. Tanja Pečnik, B. Sc.
- 24. Marko Vrabeli, B. Sc.
- Technical officers
- 25. Darko Belavič*, B. Sc. 26. Jena Cilenšek, B. Sc.
- 27 Silvo Drnovšek, B. Sc.
- 28. Brigita Kmet, B. Sc.
- 29. Milena Paiić, B. Sc.
- Technical and administrative staff 30. Tina Ručigaj, B. Sc.

Note

* part-time JSI member

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- 4. Sebastjan Glinšek, Iztok Arčon, Barbara Malič, Alojz Kodre, Marija Kosec, "Structural evolution of the KTa_{0.6}Nb_{0.4}O₃ alkoxide-based solutions: probing the transition metals local environment by X-ray absorption spectroscopy", J. sol-gel sci. technol., vol. 62, no. 1, pp. 1-6, 2012.

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- Marko Hrovat, Konrad Kiełbasiński, Kostja Makarovič, Darko Belavič, "The characterisation of lead-free thick-film resistors on different low temperature Co-fired ceramics substrates", *Mater. res. bull*, vol. 47, no. 12, pp. 4131-4136, 2012.
- 7. Jurij Koruza, Barbara Malič, Oleksandr Noshchenko, Marija Kosec, "Top-down processing of $NaNbO_3$ nanopowder", *J. nanomater.*, vol. 2012, art. no. 469143, pp. 1-7, 2012.
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- 9. Danjela Kuščer, Franck Levassort, Marc Lethiecq, Andre-Pierre Abellard, Marija Kosec, "Lead-zirconate-titanate thick films by electrophoretic deposition for high-frequency ultrasound transducers", *J. Am. Ceram. Soc.*, vol. 95, no. 3, pp. 892-900, 2012.
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- 13. Marko Pavlin, Darko Belavič, Franc Novak, "Ceramic MEMS designed for wireless pressure monitoring in the industrial environment", *Sensors*, vol. 12, no. 1, pp. 320-333, 2012.
- 14. Maja Pivko, Marjan Bele, Elena Tchernychova, Nataša Zabukovec Logar, Robert Dominko, Miran Gaberšček, "Synthesis of nanometric LiMnPO₄ via a two-step technique", *Chem. mater.*, vol. 24, iss. 6, pp. 1041-1047, 2012.
- 15. Arkadije Popović, László Bencze, Jurij Koruza, Barbara Malič, Marija Kosec, "Knudsen effusion mass spectrometric approach to the thermodynamics of Na₂O Nb₂O₅ system", *Int. j. mass spectrom.*, vol. 309, pp. 70-78, 2012.
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- 18. Tadej Rojač, Barbara Malič, Marija Kosec, Maria Połomska, Bożena Hilczer, Blaž Zupančič, Boštjan Zalar, "Mechanochemical synthesis of NaNbO₃: a complementary study of reaction mechanism using Raman spectroscopy and quadrupole perturbed ²³Na nuclear magnetic resonance", *Solid state ion.*, vol. 215, vol. 215, pp. 1-6, 2012.
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- 20. Brigita Rožič, Hana Uršič, Janez Holc, Marija Kosec, Zdravko Kutnjak, "Direct measurements of the electrocaloric effect In substrate-free PMN-0.35pt thick films on a platinum layer", In: ISIF 2012, *Integrated ferroelectrics*, vol. 140, no. 1, pp. 161-165, 2012.
- Marina Santo-Zarnik, Darko Belavič, "The effect of humidity on the stability of LTCC pressure sensors", *Metrol. Syst. Pomiarowe*, vol. 19, no. 1, pp. 133-140, 2012.
- 22. Marina Santo-Zarnik, Darko Belavič, "An experimental and numerical study of the humidity effect on the stability of capacitive ceramic pressure sensor", *Radioengineering (Prague)*, vol. 21, issue 1, pp. 201-206, 2012.
- 23. Vlasta Sedlakova, Jiri Majzner, Petr Sedlak, Martin Kopecky, Josef Sikula, Marina Santo-Zarnik, Darko Belavič, Marko Hrovat, "Evaluation of piezoresistive ceramic pressure sensors using noise measurements", *Inf. MIDEM*, vol. 42, no. 2, pp. 109-114, 2012.

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- 26. Gregor Trefalt, Barbara Malič, Janez Holc, Hana Uršič, Marija Kosec, "Synthesis of rm0.65Pb(Mg_{1/3}Nb_{2/3})O₃ – 0.35PbTiO₃ by Controlled agglomeration of precursor particles", J. Am. Ceram. Soc., vol. 95, issue 6, pp. 1858-1865, 2012.
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- 28. Hana Uršič, Jesús Ricote, Harvey Amorín, Janez Holc, Marija Kosec, Miguel Algueró, "Ferroelectric domain configurations in 0.65Pb(Mg_{1/3}Nb_{2/3})O₃ – 0.35PbTiO₃ thick films determined by piezoresponse force microscopy", *J. phys., D, Appl. phys.*, vol. 45, no. 26, pp. 265402-1-265402-11, 2012.
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PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- Andre-Pierre Abellard, Franck Levassort, Danjela Kuščer, J. -M. Grégoire, Janez Holc, Marc Lethiecq, Marija Kosec, "Electrophoretically deposited PZT thick film for high-frequency ultrasound applications", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 139-144.
- Andre-Pierre Abellard, Franck Levassort, Danjela Kuščer, Janez Holc, J. -M. Grégoire, Oleksandr Noshchenko, Marija Kosec, Marc Lethiecq, "Electrophoretic deposition (EPD) process for lead zirconate titanate (PZT) thick films fabrication and high frequency medical imaging", In: *Proceedings*, Acoustics 2012, 11ème Congrès Français d'Accoustique, [and] Annual IOA Meeting, 23-27 April 2012, Nantes, France, [S. I.], Institute of Acoustic, 2012, pp. 3331-3336.
- Ines Bantan, Breda Mirtič, Martina Oberžan, Helena Razpotnik, Danjela Kuščer, Marija Kosec, "Dense cordierite ceramics", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 -September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 351-356.
- 4. Darko Belavič, Marko Hrovat, Gregor Dolanc, Kostja Makarovič, Marina Santo-Zarnik, Janez Holc, "Design of an LTCC structure for a microceramic combustor", In: *Proceedings*, IMAPS/ACerS, 8th International Conference and Exhibition on Ceramic Interconnect and Ceramic Microsystems Technologies (CICMT 2012), April 16-19, 2012, Erfurt, Germany, [S. I.], International Microelectronics and Packaging Society, 2012, pp. 288-293.
- 5. Darko Belavič, Marko Hrovat, Kostja Makarovič, Marina Santo-Zarnik, Marjan Hodnik, Milenko Pavlović, "Benchmarking of some thick-film resistors for strain-gauge applications", In: *Proceedings*, 36th International Microelectronics and Packaging IMAPS - IEEE CPMT Poland Conference, September 26-29, Kołobrzeg, Poland, [S. l.], IMAPS-CPMT, 2012, 11 pp.
- 6. Darko Belavič, Marko Hrovat, Marina Santo-Zarnik, Marjan Hodnik, Kostja Makarovič, Vlasta Sedlakova, "Investigations of thick-film resistors for piezoresistive LTCC-based ceramic pressure sensor", In: *Proceedings*, EDS'12, Electronic Devices and Systems IMAPS CS International Conference 2012, June 28-29, 2012, Brno, Czech Republic, Ondrej Hegr, ed., Brno, IMAPS, 2012, pp. 321-326.
- 7. Darko Belavič, Marina Santo-Zarnik, Marjan Hodnik, Sandi Kocjan, Marko Stušek, Marko Hrovat, Janez Holc, Kostja Makarovič, Milenko Pavlović, "Some examples of LTCC-based ceramic pressure sensors", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 367-371.

- 8. Goran Casar, Andreja Eršte, Sebastjan Glinšek, X. Li, X. Qian, Q. M. Zhang, Vid Bobnar, "Tailoring electrically induced properties by stretching relaxor", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 210-215.
- Andreja Eršte, Barbara Malič, Brigita Kužnik, Marija Kosec, Vid Bobnar, "Equivalent circuit modeling of core-shell structured ceramic materials", In: Advances and applications in electroceramics II: [MS&T'11, Materials Science & Technology Conference & Exhibition, October 16-20, 2011, Columbus, Ohio, USA], (Ceramic transactions, v. 235), K. M. Nair, ed., Shashank Priya, ed., Hoboken, Wiley, 2012, pp. 23-29.
- Raluca C. Frunza, Marko Jankovec, Martin Strojnik, Barbara Malič, Marija Kosec, "Electrical properties of Ta₂O₅-rich dielectric thin films from solution", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 381-386.
- 11. Sebastjan Glinšek, Dmitri Nuzhnyy, Jan Petzelt, Barbara Malič, Stanislav Kamba, Viktor Bovtun, Martin Kempa, Volodymyr Skoromets, Petr Kužel, Ivan Gregora, Marija Kosec, "Broadband dielectric properties of KTaO₃ ceramics", In: *Book of abstracts*, 7th International Conference on Microwave Materials and Their Applications, MMM-201, 3-6 June, 2012, Taiwan, [S. l., s. n.], 2012, pp. 116-117.
- 12. Marko Hrovat, Darko Belavič, Kostja Makarovič, Janez Holc, "Thickfilm piezoresistors - benchmarking of LTCC substrates", In: *Power electronics: conference programme and extended abstracts*, ISSE 2012, 35th International Spring Seminar on Electronics Technology, May 9-13, 2012, Bad Aussee, Austria, Manuela Franz, ed., Johann Nicolics, ed., Vienna, Department of Applied Electronic Materials, Institute of Sensor and Actuator Systems, University of Technology, 2012, 5 pp.
- Marko Hrovat, Darko Belavič, Kostja Makarovič, Janez Holc, "Thickfilm piezorezistors as pressure sensors on different LTCC structures", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 375-379.
- 14. Jurij Koruza, Jenny Tellier, Barbara Malič, Marija Kosec, "Phase transitions of the NaNbO₃ submicron-sized powder between room temperature and 700²³C", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 247-253.
- 15. Alja Kupec, Barbara Malič, Marija Kosec, "Environmental fiendly potassium sodium niobate based thin films from solutions", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 254-260.
- 16. Kostja Makarovič, Raúl Bermejo, Irina Kraleva, Janez Holc, Marko Hrovat, Andreja Benčan, Marina Santo-Zarnik, Darko Belavič, Marija Kosec, "Mechanical properties of low-temperature Co-fired ceramics fired at different temperatures", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 297-301.
- 17. Kostja Makarovič, Anton Meden, Marko Hrovat, Janez Holc, Andreja Benčan, Aleš Dakskobler, Darko Belavič, Marija Kosec, "The effect of the firing temperature on the properties of LTCC", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 261-267.
- 18. Kostja Makarovič, Anton Meden, Marko Hrovat, Janez Holc, Andreja Benčan, Aleš Dakskobler, Marija Kosec, "The effect of phase

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ENGINEERING CERAMICS DEPARTMENT

K-6

The Engineering Ceramics Department is the leading group in the field of structural ceramics and ceramic technologies in Slovenia. The research programme comprises phenomena relevant to materials synthesis and component fabrication as well as mechanisms leading to the degradation of engineering and bio-ceramic structures under operating conditions. The applied research work is focused on new applications of engineering ceramics, the development of novel, high-strength, wear-, corrosion- and/or heat-resistant materials and the development of alternative, cost-effective and environmentally friendly ceramic technologies.

For more than two decades our group has been traditionally involved in studying the phenomena of AlN powder hydrolysis in aqueous environments, and the year 2012 was no exception. What attracts us to these studies is that the hydrolysis is a drawback on one hand, because it prevents aqueous powder processing, while on the other, it offers various interesting potentials for exploitation. The work that was already described in detail in last year's report was successfully published in highly ranked scientific publications. A detailed mechanistic model for aluminum Head: hydroxide formation during the hydrolysis in diluted aqueous AlN suspensions in a broad temperature range was **Prof. Tomaž Kosmač** published in Crystal Growth & Design. The work about the modification of the carrier Al₂O₃ powder with a high surface area, synthesized by exploiting the hydrolysis via an in situ, sol-gel reaction, to attach TiO, nanoparticles, vielding a nanostructured, γ -Al₀,/TiO₂ composite powder and a 2.7-times-higher photo-activity in the near-UV region compared to commercially available TiO, was published in Materials Research Bulletin. Recently, we

investigated the impact of cold water (5 °C) on the hydrolysis and obtained some interesting results. Namely, the results revealed that throughout the 312-hours-long hydrolysis at 5 °C the pH value of the suspensions was below 9, where the hydrolysis remained in the induction period and was eventually

suppressed due to the formation of a few-nanometers-thick film of amorphous aluminum hydroxide gel around the AlN particles, acting as a passivation layer. This process is thought to be very similar to aluminum corrosion in water. Moreover, the astonishing discovery is that the aqueous part of the suspension possessed a remarkably high value of dissolved [Al(III)]_a, being an order of magnitude higher at a given pH than the aqueous AlCl₂ solu-

tion. These findings could well prove to be beneficial for the processing of AlN in aqueous environments, as well as providing us with a new source of saturated aluminum species solution. The work was accepted in the Journal of American Ceramic Society and will be published in 2013.

In the frame of the research on thermoplastic ceramic suspensions the removal of the binder from a low-pressure injection-molded part was also investigated in 2012. A previously developed theoretical model was applied to characterize a new wick-debinding procedure in which a new extraction material is used. This material, a high-purity carbon black, has proven to be an excellent capillary extraction agent. In addition we developed a theory for describing the yield stress of paraffin ceramic suspensions in the range 40-60 vol% of powder content, taking into account the particle size distribution, type of material and the distance between the particles in the suspension. The research led to the successful defence of a PhD thesis by a young researcher from industry and the publication of an article in *the* Journal of American Ceramic Society.

In the field of electrically conductive ceramic composites, in 2012 we finished our research on the synthesis and properties of composites based on silicon nitride (Si₂N₄) with dispersed titanium nitride (TiN) and zirconium

The department had three Slovenian patents granted in 2012.



Figure 1: The defects on the surface of the Y-TZP dental ceramics due to sandblasting. The red circle marks the surface crack and the yellow circle marks the alumina sandblasting particle embedded in the surface.

nitride (ZrN) particles. The results were used for the preparation of a patent application and this year the patent for the one-step process of manufacturing a composite ceramic heater was granted. In this field, new research on electrically conductive oxide engineering ceramics based on zirconia was started in the frame of a diploma work. Namely, zirconia is a versatile oxide ceramic material with outstanding properties, which is useful in many applications. One of the major problems in the use of zirconia is the very expensive final machining. The aim of the work

was to prepare a ZrO₃/TiN electro-conductive ceramic composite, which can be machined by an electrical discharge. The electro-conductive composite based on zirconium oxide with dispersed nanoparticles of titanium nitride by the controlled precipitation of titanium hydroxide followed by calcination of the obtained powder mixture which was than thermochemically converted via titanium oxide to titanium nitride by a nitridation process was successfully prepared. The impact of the quantity and size distribution of the conducting phase on the concentration, density and electrical conductivity was investigated. The spark-plasma sintering technique was used in order to prepare dense and homogeneous ZrO2-TiN composites. We studied the influence of the sintering conditions on TiN grain growth. Moreover, the impact of the content and size of the conductive particles on the densification process and the final mechanical and electrical properties of the composites was also studied.

In the field of research on **dental ceramics** some of the major problems concerning the production of fullceramic dental contours with tetragonal zirconia (Y-TZP) as a core material, their cementation and their behaviour in clinical conditions were investigated. In the chemically aggressive environment of the oral cavity the dental

In 2012 two young researchers from the **Engineering Ceramic Department successfully** finished their PhD studies.

prosthesis products are exposed to cyclic mechanical and thermal loads, that with time weaken the core ceramic material as well as the strength and stability of the connection joints. Since because of the high chemical stability of zirconia these connections are not very strong in the first step we investigated the influence of the nanostructured aluminate coating on the bonding strength of the dental cements to dental ceramics based on

Y-TZP and Ce-TZP/ Al_2O_3 . The coatings, which do not damage the surface, were prepared by the precipitation of aluminium hydroxides formed during the hydrolysis of the AlN powder in water. After the thermal treatment these coatings have a uniform thickness and are homogenous, have a very high specific surface area and are strongly bonded to the ceramic surface. The results of the adhesion measurements showed that the aluminate coating improves the bonding strength by more than 100 %, while the strength is retained even after thermocycling of the samples, which is not the case with the samples without the coating. These samples spontaneously debonded during the thermocycling test. These results were published in the Journal of European Ceramic Society. The research of phase instability of conventionally sintered dental 3Y-TZP ceramics in simulated clinical conditions was also continued. Two commercially available granulates of Y-TZP powder with the same chemical composition but different size of primary crystallites and specific surface area were used. By changing the sintering temperatures

a series of samples were prepared that varied in the grain size, mechanical properties and transformability. The samples were exposed to accelerated ageing in deionised water at 134 °C and the zirconia phase transformation from tetragonal to monoclinic was monitored with regard to ageing time. The thickness of the transformation zone and the influence of ageing on the mechanical properties were investigated. Also, this research was published in the Journal of European Ceramic Society.

In the frame of the PhD study of a young researcher from the Medical Faculty the influence of kinetic energy (or momentum) of the impact particles on the type of damage during the sandblasting of the two types of dental ceramics differing in the grain size were studied. The conditions at which the surface cracks appeared on the surface were determined and it was explained why there is a difference between the fine- and coarse-grained material. The work was presented in an introductory lecture at the Conference of the American Association for Dental Research (AADR).

The research on porous yttria-stabilized tetragonal zirconia (Y-TZP) ceramics for dental applications with a substantially lower elastic modulus while preserving a useful strength for applications in dental medicine was successfully finished with the defence of a PhD thesis by a young researcher. With this concept, we tried to reduce the mismatch between the elastic proper-

ties of ceramic prosthetic products and tooth substance that can, during loading, lead to significant elastic stress, which, according to the literature, is one of the possible causes for the shorter life of dental prosthetic substitutes in the mouth. The research was published in the Journal of European Ceramic Society.

The influence of the strength of the ceramic skeleton on the strength of a glass-infiltrated ceramic composite was investigated in a diploma thesis. The ceramic skeleton was prepared using the HAS process that enables the preparation of moderately porous alumina ceramic with improved mechanical strength at an equal relative density compared to a ceramic prepared using traditional shaping processes. After the glass infiltration a higher strength of the composites was achieved, if compared to commercially available glass infiltrated composites used for the production of dental crowns and bridges. The research showed that the strength of the composite depends on the

Figure 2: FEG-SEM image of calcium phosphate crystals on the surface of zirconia substrate after thermal treatment.



strength of the ceramic skeleton and the amount of the infiltrated glass. With this we indicated the direction of the development of glass-infiltrated ceramic composites used in dental medicine.

The research on the synthesis of bioactive calcium phosphate coatings on zirconia Y-TZP ceramics, which is due to its aesthetic and mechanical properties, frequently used in medicine as a material for dental implants were continued in 2012. The fixation of an implant can be improved if its surface is covered by a bioactive calcium phos-

phate coating that forms a strong bond with the bone tissue. The coatings were prepared using a biomimetic method in which the ceramic substrate is immersed in a solution with the same physiological temperature and similar composition as human blood plasma. The advantages of this bio-mimetic method are its simplicity, low price and good control of the composition of the coatings. One of the main problems that restrict the use of bio-mimetic coatings in medicine is the poor adhesion of coatings to the substrate, so in the research we primarily dealt with ways of improving the mechanical properties of the coatings. It was found that the thermal treatment improved the adhesion of coatings and at the same time it enables us to control their phase composition. Thus, we have developed procedures for the synthesis of calcium phosphate coatings with different phase composition (hydroxyapatite, octacalcium phosphate, β-tricalcium phosphate), different morphology and mechanical properties. The procedure was described in an article published in the journal Applied Surface Science. Especially important is a new procedure for the synthesis of thin β-tricalcium phosphate coatings with very good mechanical properties. Mechanical tests showed that the adhesion of such coatings is comparable or even better than the adhesion of calcium phosphate coatings on commercially available bone grafts.

In 2012, the research on the improvement of wear resistance of Figure 3: All of the results of the measurements of bending strength of titanium alloys used for the preparation of bone implants was finished. By nitridation at elevated temperatures (600-900 °C) in an ammonia atmos-



alumina ceramics from the Hidria AET company.

phere, we successfully prepared a 100- to 300-nm-thick layer of titanium nitride on the surface of metallic titanium or its alloys. This has significantly increased the surface hardness and, consequently, improved the wear resistance of the material. The application of titanium nitride layers on the surface of metals to increase hardness and thereby improve the wear resistance is known and often used especially in the case of the manufacture of various cutting

tools. Despite this, the major problem is the adhesion of the layer applied to the metal, which is in the case of medical applications even more important. In our study the adhesion between the nitride layer and the metal was tested with a "scratch" test, which showed that the adhesion between the coating

prepared by nitriding in ammonia is better than in the case of a TiN coating using the PVD method. The wear rate of titanium and its alloys, in which we deposited TiN layer with PVD method and were previously nitrided in the atmosphere of ammonia, was reduced by two-thirds.

For the company Eternit AG from Switzerland a feasibility study of the production of fibre-reinforced materials based on fly-ash geopolymers was conducted. It was shown that this secondary raw material could be successfully used for the production of composite panels that achieve comparable mechanical properties as plates made from fibre-cement composites.

In cooperation with Hidria AET we prepared and characterized Al₂O₂/ZrO₂ composite materials using a process of low-pressure injection moulding of paraffin suspensions, where we used a new and economical way to prepare ZrO, powders. With a relatively small addition of ZrO, one could significantly improve the mechanical properties of Al₂O₂ ceramics for applications at room temperature and at the same time the price of raw materials would not significantly increase. We also continued with a statistical analysis of data for the strength of ceramic samples that were available in a very large number of measurements of flexural strength. A large set of experimental values was used, in cooperation with foreign researchers, to verify their hypotheses. Research has shown that with the use of the so-called best method of assessing the likelihood we can improve the accuracy of the determination of the Weibull distribution parameters.

Some outstanding publications in the last three years

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In 2012 we cooperated with many research institutions and industrial partners.

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- 3. Lovro Gorjan, Aleš Dakskobler, Sintering heat treatment procedure of formpieces, SI23763 (A), Urad RS za intelektualno lastnino, 31.12.2012.
- 4. Aljoša Maglica, Kristoffer Krnel, Tomaž Kosmač, Single-stage process of manufacturing a composite ceramic heater, SI23609 (A), Urad RS za intelektualno lastnino, 31.7.2012

INTERNATIONAL PROJECTS

- Alternative binders for building materials preliminary study Eternit (schweiz) AG Prof. Tomaž Kosmač
- 7. FP MICROFLEX: Micro fabrication production technology for MEMS on new emerging smart textiles/flexibles European Commission
- Prof. Tomaž Kosmač, Prof. Marija Kosec
- 7. FP CERAMPOL: Ceramic and polymeric membrane for water purification of heavy metal and hazardous organic compound
 Prof. Tomač Kogemeč Acet. Prof. Daniela Kuščer Heavatin

Prof. Tomaž Kosmač, Asst. Prof. Danjela Kuščer Hrovatin

VISITORS FROM ABROAD

- 1. Dr. Hans Musch, Eternit (Schweiz) AG, Research and Development, Niederurnen, Switzerland, 18. 1. 2012, 4. 4. 2012
- Prof. Michael V. Swain, Biomaterials Unit, Faculty of Dentistry, University of Sydney, National Innovation Centre, Australian Technology Park, Eveleight, Australia, 25. 9.–12. 10. 2012

RESEARCH PROGRAM

1. Engineering and bioceramics Prof. Tomaž Kosmač

R & D GRANTS AND CONTRACTS

- 1. Research of dental ceramics Prof. Tomaž Kosmač
- Ceramic materials for 3D structures and study of functional properties Prof. Tomaž Kosmač
- Prof. Mutlu Özcan, University of Zürich, Center for Dental and Oral Medicine, Zürich, Switzerland, 19. 10. 2012

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- 4. Dr. Andraž Kocjan, on postdoctoral leave since 01.06.12
- 5. Dr. Irena Pribošič, left 01.12.12
- 6. Dr. Krunoslav Vidović*, left 01.07.12
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- 8. Dr. Sebastjan Perko, left 01.06.12

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PATENT APPLICATION

1. Aleš Dakskobler, Andraž Kocjan, Manca Logar, *Method for the preparation of carrier colloidal powder with high specific surface area*, W02012053990 (A2), World Intellectual Property Organization, 26.4.2012.

PATENT

- 1. Aleš Dakskobler, Andraž Kocjan, Manca Logar, *Method for the preparation of carrier colloidal powder with high specific surface area*, SI23502 (A), Urad RS za intelektualno lastnino, 30.4.2012.
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- Lovro Gorjan, Aleš Dakskobler, Sintering heat treatment procedure of formpieces, SI23763 (A), Urad RS za intelektualno lastnino, 31.12.2012.
- Aljoša Maglica, Kristoffer Krnel, Tomaž Kosmač, Single-stage process of manufacturing a composite ceramic heater, SI23609 (A), Urad RS za intelektualno lastnino, 31.7.2012.



MENTORING

- 1. Lovro Gorjan, *Debinding of low-pressure powder injection-molded parts:* doctoral dissertation, Ljubljana, 2012 (mentor Tomaž Kosmač).
- 2. Sebastjan Perko, *Moderately porous zirconia ceramics for dental applications:* doctoral dissertation, Ljubljana, 2012 (mentor Tomaž Kosmač; co-mentor Aleš Dakskobler).

DEPARTMENT FOR NANOSTRUCTURED MATERIALS K-7

The basic and applied research in the Department for Nanostructured Materials includes ceramic materials, metals, intermetallic alloys and minerals. Our research encompasses conventional processing as well as the development of new technologies and methods for preparing new materials with novel properties. It includes experimental and theoretical investigations of structures, analyses of chemical compositions at the atomic level, and measurements and calculations of physical properties, all of which help us to improve the properties of micro- and nanostructured materials.

In 2012 we were awarded the EU FP7 project "Replacement and Original Magnet Engineering Options" (RO-MEO) in which we are the coordinator and an active research group in grain-boundary engineering (GBE) and the characterization of magnets using magnetic-properties measurements and high-resolution electron microscopy on the nano and atomic levels. The project has two goals: firstly, decreasing and/or completely avoiding the use of heavy rare earths in Nd-Fe-B high-energy magnets and, secondly, inventing new magnets that will have properties between ferrites and high-energy magnets based on rare earths and transition metals.

We began to work on another EU FP7 project, Nanocrystalline Permanent Magnets Based on Hybrid Metal- Prof. Spomenka Kobe Ferrites (NANOPYME), which will focus on developing new permanent-magnet materials that fill the gap between conventional ferrite magnets and high-energy, rare-earth-based Nd-Fe-B and Sm-Co-based magnets. The department is responsible for producing nanoscale powders and for technology transfer to industry.

As part of our work on improving the corrosion-resistance properties of bonded and injection-moulded rare-earth-based magnets we have coated Nd-Fe-B melt-spun powders with SiO₂ and Al₂O₂ using the sol-gel technique. Highly accelerated stress tests were conducted to compare the corrosion properties of the ribbons. The compositions and microstructures of the ribbons and surface layers were determined by AES, XPS, Raman spectroscopy, SEM and EDS. The magnetic properties were measured with a vibrating-sample magnetometer. Both the SiO₂ and Al₂O₃ coatings resulted in superior corrosion resistance and magnetic properties. This technique should expand the range of use of Nd-Fe-B bonded magnets to applications with temperatures as high as 110 °C and 90% humidity.

Our work on the hydrogenation of amorphous rare-earth-based hard-magnetic amorphous materials was focused on studying the effects of a range of hydrogen pressures and temperatures on the magnetic and structural changes in Nd-Fe-Al alloys with compositions close to Nd₆₀Fe₂₀Al₁₀, using vibrating-sample magnetometry, x-ray diffraction and transmission electron microscopy.

In collaboration with the Department for Inorganic Chemistry we managed to coat Nd-Fe-B melt-spun ribbons with a thin (3 nm) layer of DyF₄ using an innovative fluorolythic sol-gel reaction with Dy-isopropoxide as a precursor. The powder will be used as a basic material for bonded magnets with improved coercivity.

Nano-dimension, intermetallic, hard magnetic systems of Fe-Pd and Co-Pt were electrodeposited and investigated for their magnetic shape memory (MSM) effect ($Fe_{7a}Pd_{2a}$) in a national project with the NIC and as part of an MNT-ERA-NET project, and due to their potential for use in perpendicular recording (Co-Pt). Since the MSM effect is composition sensitive, an electrochemical kinetic study of the Fe-Pd deposition was made on flat and porous templates. It was found that the deposition of both ions is irreversible and diffusion controlled, with the diffusion and kinetics being faster on the flat electrode. Based on the obtained parameters pulsed-plated conditions for achieving Fe₇₀Pd₂₀ nanowires with constant composition were proposed. Deposited Fe₇₀Pd₂₀ nanowires had a face-centred tetragonal crystal structure, which was successfully transformed to a face-centred cubic structure via thermal annealing and quenching, which is the basis for the MFM effect. For the biomedical purposes the Fe-Pd nanowires were additionally coated with SiO₂, which increases their functionality. Co-Pt nanowires with different (marked by arrow). Transmitted light microscopy, crossed polars.

In 2012 we began our role as coordinators of the EU FP7 project "Replacement and Original Magnet Engineering Options" (ROMEO). The project aims to reduce the dependence of European industry on expensive and erratic supplies of rare-earth raw materials, primarily from China.

We successfully used electrophoretic deposition as a method to effectively coat the surface of a Nd-Fe-B sintered magnet with Dy(Tb)F₃ powder and achieve 30 % higher coercivities with an optimized amount of expensive heavy rare earth (Fig. 4).

Figure 1: Meteorite Jesenice. (a) Typical porphyritic olivine chondrule and (b) porphyritic olivine chondrule containing relict olivine grain





DLC+hydroxy acid DLC+benzene Figure 2: Bond formation between the surface of a doped DLC and hydroxy acid or benzene.

aspect ratios were electrodeposited into porous alumina templates. It was found that the direction of the magnetization easy axis can be tailored from parallel to perpendicular, taking into account all the involved anisotropies. The magnetic force microscopy study revealed that by increasing the aspect ratio, the Co-Pt system transforms from a mono-domain to a multi-domain structure, leading to a coercivity reduction for high aspect ratios. The ability to tailor the easy magnetization axis direction finds applications in perpendicular recording, since more information can be stored in a perpendicular geometry.

In our research on **magnetocaloric materials** based on $\text{Gd}_5(\text{Si},\text{Ge})_4$ we found that the microstructure has a large effect on the magnetic properties. The orthorhombic-monoclinic structural change, which occurs under the influence of an external magnetic field, usually happens at a field below 1

Tesla. If we modify the microstructure with small substitutions of iron and fast cooling of the melt, we modify the microstructure in such a way that the structural change occurs at higher magnetic fields. It was also found that for a correct calculation of the magnetic entropy change from the magnetic data one has to use thermo-magnetic data measured at a constant magnetic field.

In the research on intermetallic magnetocaloric materials based on amorphous iron alloys with added transition



Figure 3: The SITE-SiCf/SiC plate

metals we want to achieve a compromise between a high magnetocaloric effect and a low magnetic ordering temperature. Adding metals usually increases the magnetocaloric effect, but also increases the magnetic ordering temperature much above room temperature. We focused our research on adding nickel to the alloy $Fe_{89}Ni_xZr_{10}Cu$ (x=0-8) and achieved a remarkable increase in the magnetocaloric effect with a modest increase in the magnetic ordering temperature.

 MgH_2 -based systems have the highest potential to be used as hydrogen storage material. The DOE goal for 2015 is 4.5 wt.% of H, whereas pure MgH_2 yields 7.6 wt.%. However, the sorption kinetics is very slow, which restricts its application either in hydrogen fuel-cell powered vehicles or NiMH batteries. Therefore, numerous attempts are performed worldwide to improve sorption kinetics by the addition of various dopants, i.e., pure transition metals (and rare earths) in nano-from, their alloys, oxides, carbides and halogenides, via surface modification using gentle planetary milling in order to achieve a catalytic effect. Most of these additives improve the sorption kinetics and as expected lower the capacity, as well. Nevertheless, to the

best of our knowledge there are no reports in the literature about using quasicrystals of any kind or any system for this purpose. Thus, we prepared icosahedral Ti-Zr-Ni-based quasicrystals and mixed them with commercial MgH_2 and ball-milled the mixture for several hours. In parallel, we milled pure MgH_2 in order to eliminate the effect of particle size reduction on the kinetics. Using mass spectrometry we found a 60°C lower temperature of hydrogen desorption after 36 hrs of milling in the case when (5 wt.%) quasicrystals were used as compared to pure MgH_2 .

Within the European fusion programme, in which we have already collaborated for eight years, the most important result is the optimisation of the SITE-P process developed in our laboratory. The process involves the electrophoretic infiltration/ deposition of SiC powder to fill the voids within the SiC-fabric and enables the fabrication of a 3-dimensional SiCf/SiC composite for the firstwall blanket in future fusion-power plants. In 2012 we modelled the absorption molecules present in lubricants at the DLC surface and found that the strongest bonds were formed between the metallic dopants from the DLC and the oxygen atoms from the molecule COOH or OH groups (Fig. 2). On the basis of *ab-initio* calculations we determined the most probable muon stopping-sites in some complex magnetic systems. We also worked on the implementation of the densitymatrix-renormalization-group method (DMRG).

Within the European fusion programme, in which we have already collaborated for eight years, the most important result is the optimisation of the SITE-P process developed in our laboratory. The process involves the electrophoretic infiltration/deposition of SiC powder to fill the voids within

the SiC-fabric and enables the fabrication of a 3-dimensional SiC_f/SiC composite for the first-wall blanket in future fusion-power plants. We demonstrated the possibility of up-scaling the process and have fabricated a set of samples for mechanical characterisation. Special attention was paid to an increase in the thermal conductivity of the composites by microstructural control. As a result, high values were achieved, i.e., 60 W/mK at room temperature and 30 W/mK at 1000 °C, which places the SITE-SiC/SiC among the best related materials (Fig. 3).
Electrophoretic deposition was also used in the fabrication of a SiC-based ceramic composite reinforced with carbon nanotube (SiC-CNT), where we achieved a homogeneous distribution of CNT within the ceramic matrix. A comprehensive study of the electrokinetic properties of suspensions also resulted in the successful electrophoretic

deposition of bulk parts of thermoplastic polymer polyether-ether-ketone (PEEK), which is a topic of research in collaboration with the Mechanical Engineering Faculty, University of Ljubljana. The same process has also been tested as a method for coating metallic gears with PEEK (collaboration with the Mechanical Engineering Faculty, University of Maribor).

In the frame of research of materials for use in medicine, we continued the study of the properties of TiO₂ coating on a Ti₆Al₄V alloy formed by a hydrothermal treatment of the alloy. It was confirmed that the thin crystalline (anatase) coating significantly reduces the leaching of aluminium and vanadium ions from the alloy, improves the wetting and contributes to improved bone attachment. Special attention has been paid to the photocatalytic properties in correlation with the bacteriostatic behaviour (BioTiNet, FP7-ITN).

Results of the research of bioactive glass, which was developed within the scope of the FP6-IP-SME project "Meddelcoat", have been published in International Orthopaedics, where the observed beneficial effect of a bioactive glass coating on a metal implant on osseointegration was presented. The research of bioactive glass was also carried on within an informal collaboration with Educell d.o.o., where bioactive glass has been studied as a candidate material for use in bone-tissue engineering regeneration. The effect of powder and sintered bioactive glass on cells has been evaluated and compared. In addition, research with bioactive glass in the form of a paste or gel for the reduction of dentine hypersensitivity after professional teeth bleaching was started as an informal collaboration with Dental Studio (Fig. 5).

Within the frame of the COST action NAMABIO "From nano to macro biomaterials (design, processing, characterization, modelling) and applications to stem cells regenerative orthopaedic and dental medicine" a collaboration was established with a world-leading research group in the field of tissue engineering at the University of Minho in Portugal. A set of biodegradable Figure 4: Core-shell structure of the grains in Nd-Fe-B magnets and and bioactive nano-composite scaffolds was prepared and characterised. The WDS analysis, which shows the Tb distribution that contributes to the composite scaffold, supposed to be used as a cell-support in the regeneration of large osteochondral defects, is composed of natural polymer (gellan gum)





coercivity improvement of 30%.

reinforced with nanoparticulate bioactive glass powder. With the addition of bioactive glass we achieved bioactivity (precipitation of hydroxyapatite in body fluid) and favourable biodegradation, which are both important for new bone formation. A significant improvement of the mechanical properties was also observed: Young's modulus was five times higher for the composite material than for biopolymer material alone. This is ascribed not only to the presence of particles but also to the increased concentration of calcium ions, allowing the more intensive crosslinking of monomer gellan gum molecules (Fig. 6).

In the field of ZnO-based varistor ceramics we studied the influence of the Bi₄Ti₃O₁₂ (BIT) addition on grain growth and microstructure development. A homogeneous microstructure development was achieved during the rapid release and efficient distribution of TiO,, which triggered the formation of inversion boundaries (IBs) in ZnO grains. It can be achieved by instant decomposition of the BIT to TiO₂-rich Bi₂O₂ liquid phase in samples suddenly exposed to temperatures above 1100°C. The results are important for the development of varistor ceramics with very low breakdown voltages below 50V/mm.

The development of thick-film varistors was focused on studying the influence of organic vehicles and the amount of added varistor powder filler on the rheological characteristics of pastes and their screen printing performance.

Simple and cheap low-temperature hydrothermal synthesis at 90°C enabled the preparation of ZnO films with high optical transparency over 80% and a low resistivity. For the growth of a smooth, dense and highly (0001) oriented polycrystalline ZnO film from a solution of Zn-nitrate during the addition of Na-citrate a proper nucleation layer of ZnO on glass is required. The formation of a ZnO nucleation layer and the influence of its characteristics on the growth and optical properties of the ZnO films were studied. A highly homogeneous and continuous nucleation layer of well-connected ZnO grains with sizes from 30 to 100 nm, which enable the hydrothermal growth of a highly transparent ZnO film, can be prepared from a Zn-acetate layer with a thickness of at least 90 nm at temperatures of calcinations between 350 and 600°C. The higher is the number of the ZnO nuclei per unit area, the thinner the

ZnO film with higher density, superior (0001) orientation and hence higher transparency can be obtained in hydrothermal growth. At lower thicknesses of Zn-acetate layer and higher calcination temperatures a discontinuous nucleation layer formed from larger and separated ZnO grains, resulting in a poorly textured and porous ZnO film with a low optical transparency. Economical ZnO films can replace transparent-conductive ITO (In-Sn-O) films with rare and hence expensive In, which nowadays dominates in technologies of flat-panel displays and solar cells.

We continued with a study of the nucleation and crystallization of **ZnO nanoparticles** using electron microscopy and SAXS (small-angle X-ray scattering) and explained the mechanisms of crystallization and the transformation of zinc-hydrocincite to zinc oxide.



Figure 5: a) Open dentin tubules causing dentin hypersensitivity and b) dentin tubules closed due to the re-mineralization after treatment with bioactive glass.

In collaboration with the company VARSI we continued the development of nano-varistors and special varistors with a high stability of leakage current under a dc field for applications in the overvoltage protection of renewable energy systems (solar panels and wind-turbine generators).

The development of oxide **thermoelectric materials** of n-type was focused on studying the influence of composition and firing temperature on the formation of the phases in the (ZnO)_xIn₂O₃ homologous series, microstructure, structure and consequently thermoelectric characteristics. In the development of p-type thermoelectric materials the preparation of highly textured samples of Ca₃Cu₄O₉ compound was studied and its synthesis using spark plasma sintering (SPS) method. A Z-meter was constructed for

measurements of the thermoelectric characteristics up to a temperature of 1000K. The first test measurements of our samples up to temperatures of 750°C were made and the obtained results are comparable with the results obtained on commercial instruments.

Within the investigation of other potential thermoelectric materials we synthesized n-type thermoelectrics based on SrTiO₃, Sr₂TiO₄ and Sr₃Ti₂O₇ doped with different amounts of Nb₂O₅ in Gd₂O₃. We expect that the incorporation of dopants will beneficially increase the electrical conductivity of these perovskite-based ceramics. Additionally, by controlling the intergrowth of Ruddlesden-Popper layers within the perovskite matrix in non-stoichiometric Sr₂TiO₄ and Sr₃Ti₂O₇ we intend to reduce the thermal conductivity.

The synthesis of perovskite $BaTiO_3$ nanorods via sol-gel electrophoretic deposition into anodic aluminium oxide (AAO) membranes has proven to be very successful and useful. When measuring the electrical properties

In the article "Characterization of Individual Barium Titanate Nanorods and Their Assessment as Building-Blocks of New Circuit Architectures" we reported on the integration of individual BaTiO₃ nanorods into simple circuit architectures. At the beginning of 2012 this work received the title of "Best journal highlights articles". of BaTiO₃ nanorods we have come up with interesting scientific findings, which were published in the journal Nanotechnology. In the article "Characterization of Individual Barium Titanate Nanorods and Their Assessment as Building-Blocks of New Circuit Architectures" we reported on the integration of individual BaTiO₃ nanorods into simple circuit architectures. At the beginning of 2012 this work received the title of "Best journal highlights articles". The Slovenian journal Finance also published an article on the **BaTiO₃** humidity nanosensors.

We continued the study of nucleation and synthesis of **titania nanoparticles** in anatase and rutile crystal form and thin-titania films on metal

substrates using hydro and solvothermal methods. The influence of process parameters (the used solvents were water, isopropoxide, glycerol, etc.) on the size, morphology and photocatalytic efficiency of particles and thin films were



Figure 6: Wall of composite scaffold (left) and hydroxyapatite on the composite as evidence of bioactivity (right).

studied. We were able to tailor the morphology of titania nanoparticles in the form of rods, bipyramids, stars, flowers, sea-urchins, etc. The explanation of the nucleation and growth of anatase particles to the specific morphologies were published in Journal of Crystal Growth.

In the field of photovoltaics we assembled and tested the semi-flexible DSSC (dye-sensitized solar cells) solar cells. For the flexible substrate the titanium foil was used and anodized. The produced thin oxide layer of 2-D ordered TiO, nanotubes serves as an active component of DSSC cells.

We optimized the parameters for the anodization of aluminium foil and alloys. The obtained oxide layer was coloured by the selected ion. In the case of copper ions we get ampurple colour of the oxide layer. This work is a cooperation with the department of thin films and surfaces (F3) and Impol industry within an ARRS project.

In collaboration with colleagues from Department of Materials Physics, Montanuniversität Leoben and Erich Schmid Institute of Material Science, Austrian Academy of Sciences, Leoben, Austria a systematic study of the effect of focused ion beam (FIB) fabrication on the mechanical properties of miniaturized mechanical tests by means of advanced analytic and *in situ* transmission electron microscopy (TEM) was performed. This study deals with the influence of a few nanometre sized crystal defects on the mechanical properties of miniaturized components. Although the formation of these defects is unwanted, they represent an inevitable side effect in the material manipulation by the focused ion beam, a very common technique used worldwide, especially in microelectronics. Through a combination of mechanical and atomic-resolution analytical techniques a mechanism was determined on how these defects degrade the material properties, but much more important a suitable heat treatment was established that can drastically reduce the amount of such defects, which provides an extremely usefully procedure for the material healing. This work was published in Philosophical Magazine. The importance of the study of the effect of FIB fabrication on the mechanical properties of miniaturized mechanical tests by means of advanced analytic and *in situ* TEM was recognized by the Austrian Society for Electron Microscopy by awarding the associated paper with the **Fritz Grasenick Award 2012**, which represents the highest national award in the field of electron microscopy.

In collaboration with the University of Ljubljana, NTF, Department of Geology systematic electron microscopy studies of the meteorite Jesenice were initiated. Meteorite Jesenice (3.61 kg), which hit Slovenia in 2009 represents the most preserved stony meteorite - chondrites in Slovenia and probably also in Europe, which provides an unique opportunity for better understanding of the formation and the evolution of our Solar system in the period of \sim 4.6 billion years ago. As a result of first studies, interestingly, inside one of the chondrula a relict crystal grain composed of olivine mineral was found. Relict is a possible remnant of previous generation of chondrules, which can date even before the existence of our Solar system and therefore represents one of the oldest if not the oldest object ever found on our planet (Fig. 1).

The importance of the study of the effect of FIB fabrication on the mechanical properties of miniaturized mechanical tests by means of advanced analytic and *in situ* TEM was recognized by the Austrian Society for Electron Microscopy by awarding the associated paper with the Fritz Grasenick Award 2012, which represents the highest national award in the field of electron microscopy.

We characterized semiconducting BiSe, Bi_2Se_3 and PbSe obtained by mechanochemical synthesis for applications in optoelectronic devices. In our latest research work we focused on the MgO-Al_2O_3-BeO ternary system. The two end-members of this system - MgAl_2O_4 spinel and BeAl_2O_4 chrysoberyl - are both well-known and technologically interesting materials, whereas the ternary Be-Mg-Al oxides (taaffeites) are recognized mainly in the geological community as naturally occurring precious minerals. In our experimental work we directly revealed for the first time that twinning in MgAl_2O_4 is chemically triggered by the addition of BeO and that the structure of twins is closely related to the structure of taaffeites. The nucleation and growth mechanism of twinned crystals is explained on the so-called twin-induced exaggerated grain growth theory. Our findings will be important for future

engineering of spinel-based materials. A paper on this subject is submitted to CrystEngComm.

A scientific monograph entitled **Minerals of the mercury ore deposit Idria** was published in three languages, Slovene, German and English, the latter by the renowned international scientific publisher Springer Verlag. Mineralogy is explained in terms of geological processes that were active during the formation of the ore deposit. The central part of the book is dedicated to the main mineral of the ore deposit, cinnabar. It occurs in a variety of crystal forms, of which the most special are the lateral interpenetration twins. The book is written for a broad readership, and is interesting for geologists, mineralogist and crystallographers, as well as for those interested in the history of mineral collecting in Idria.

One of the most important research areas of the group is the implementation of various electron microscopy analytical techniques within the existing EU project **ESTEEM2**, such as electron energy-loss spectroscopy (EELS), high-resolution scanning transmission electron microscopy (STEM, HAADF-STEM) electron holography and mechanical preparation of the TEM samples. The research group is additionally strongly involved in managing



Figure 7: Twin of quartz - using the electron backscatter diffraction (EBSD) method we have accurately determined the crystal orientation and so directly confirmed the presence of Japanese twin in this natural quartz crystal.

the Center for Electron Microscopy within the frame of the national infrastructure Center for Microstructural and Surface analysis. Implementation of various electron microscopy analytical techniques and the possibility for researchers to access research infrastructure for electron microscopy is of utmost importance for numerous research institutions, industrial partners, as well as for graduate and post-graduate education.

In the frame of this research we have also successfully implemented the advanced, improved methods of high-resolution scanning electron microscopy (FEGSEM) and energy-dispersive and wavelength-dispersive X-ray spectroscopies (EDS, WDS) for the materials characterization on sub-micrometre and nanometre scales, such as TiO_2 and ZnO nanoparticles, FePd and CoPt nanorods and thin films and Tb-doped NdFeB sintered permanent magnets. Using the electron backscatter diffraction (EBSD) method we have analysed the grains orientation and

texture in polycrystalline ZnO-ceramic thin films. With EBSD we have quantitatively evaluated and determined the type of twins in natural quartz (SiO₂) crystals (Fig. 7).

For industrial partners and other research institutions we have performed the analyses and expertise related to microstructural characterization of various materials in order to solve technological problems in production and/ or in the research and development of new products. The main collaborations were realized with SwatyComet Maribor, Cinkarna Celje, ITW Metalflex Tolmin, IFB Inštitut za fizikalno biologijo Ljubljana, Belinka Ljubljana, RC SIMIT Kidričevo, UL-NTF Oddelek za tekstilstvo Ljubljana, Ortopedska Bolnišnica Valdoltra Ankaran.

Some outstanding publications in the past year

- 1. Novak, S., Iveković, A.: SiC-CNT composite prepared by electrophoretic co-deposition and polymer infiltration and pyrolysis process. J. phys. chem., B Condens. mater. surf. interfaces biophys., [in press] 2012, p. 6
- Žužek Rožman, K., Pečko, D., Šturm, S., Maver, U., Nadrah, P., Bele, M., Kobe, S.: Electrochemical synthesis and characterization of Fe₇₀Pd₃₀ nanotubes for drug-delivery applications. Mater. chem. phys., 2012, vol. 133, issue 1, pp. 218-224
- Kiener, D., Zhang, Z., Šturm, S., Cazottes, S., Imrich, P. J., Kirchlechner, C., Dehm, G.: Advanced nanomechanics in the TEM: Effects of thermal annealing on FIB prepared Cu samples. Philos. mag., 2012, vol. 92, no. 25-27, pp. 3269-3289
- 4. Drnovšek, N., Novak, S., Dragin, U., Čeh, M., Gorenšek, M., Gradišar, M.: Bioactive glass enhances bone ingrowth into the porous titanium coating on orthopaedic implants. Int. orthop., 2012, vol. 36, no. 8, pp. 1739-1745
- Podlogar, M., Richardson, J. J., Vengust, D., Daneu, N., Samardžija, Z., Bernik, S., Rečnik, A.: Growth of transparent and conductive polycrystalline (0001) - ZnO films on glass substrates under low-temperature hydrothermal conditions. Adv. funct. mater. (Print), 2012, vol. 22, no. 15, pp. 3136-3145

Awards and appointments

1. Martina Lorenzetti, Saša Novak, Spomenka Kobe, 2nd best oral presentation in Young researchers section, 20th Jubilee Conference on Materials and Technology, 17.–19. 10. 2012, Portorož, Slovenia, given by the conference committee. Awarded contribution: Investigation of the properties of Titania coatings on Ti-based alloys substrates for body IMP.

Organization of conferences, congresses and meetings

- 1. The 20th Jubilee Conference on Materials and Technology, Portorož, Slovenia, 17.-19. 10. 2012 (co-organisation)
- C-MAC Days 2012, AGH University of Science and Technology, Krakow, Poland, 10.–13. 12. 2012 (membership in Science Board and General Assembly and European integrated Center for the Development of New Metalic Alloys and Compounds (C-MAC))
- Fusion Expo: Energie Fusion, Energie du futur, Faculté des Sciences et technologies, Nancy, France, 26. 1.–
 4. 2. 2012 (co-organisation)
- 4. Fusion Expo: Energie Fusion, Energie du futur, Printemps des Sciences, Centre de Culture Scientifique, Coulliet, Charleroi, Belgium, 16. 3.–20. 4. 2012 (co-organisation)
- 5. Fusion Expo, Stefan Days, Jožef Stefan Institute, Ljubljana, Slovenia, 24. 3. 2012 (co-organisation)
- 6. Fusion Expo, La Fusion, l'Energie du futur, Visiatome, CEA Marcoule UCCAP, Bagnols-sur-Cèze, France, 12. 5.-8. 7. 2012 (co-organisation)
- 7. Fusion Expo, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, 3.-14. 9. 2012 (co-organisation)
- 8. 27th Symposium on Fusion Technology 2012 SOFT, Fusion Expo, Fusion, Énergie du futur, Palais des Congrès of Liège, Belgium, 19. 9.–5. 10. 2012 (co-organisation)
- 9. Light12 event European Night of Research, Planetario e museo astronomico, Rome, Italy, 29. 9. 2012 (co-organisation)
- 10. Fusion Expo: Energia da Fusione, Per il Futuro, Festival della Scienza, Universitaria di Genova, Genoa, Italy, 25. 10.-4. 11. 2012 (co-organisation)
- 11. Fusion Expo: ITER et la Fusion, L'Energie du Futur, Aix-en-Provence, France, 13.-28. 11. 2012 (co-organisation)

Patents granted

1. Saša Novak, Nataša Drnovšek, Gregor Murn, Bone implants with multilayered coating and process of their preparation, SI23420 (A), Urad RS za intelektualno lastnino, 31.1.2012

INTERNATIONAL PROJECTS

- 7. FP ROMEO, Replacement and Original Magnet Engineering Options 1. European Commission Prof. Spomenka Kobe
- FP NANOPYME; Nanocrystalline Permanent Magnets Based on Hybrid Metal-Ferrites 2. European Commission
- Asst. Prof. Paul John McGuiness 3.
- 6. FP ESTEEM; Enabling Science and Technology through European Electron Microscopy European Commission
- Prof. Miran Čeh
 FP EURATOM; Public Information; Research Unit, Administration and Services RU-FU; Annex 3 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology
- Asst. Prof. Saša Novak Krmpotič 7. FP - EURATOM; Development of Beta SIC Fibres with W Core - 4.1.1.1.-FU; Annex 2 to 5 Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology
- Asst. Prof. Goran Dražić 7. FP - BioTiNet; Academic-Industrial Initial Training network on Innovative Biocompatible Titanium-based Structures for Orthopaedics European Commission
 - Prof. Spomenka Kobe
- 7. FP 2020 Interface; Nanoscale of Tribological Interfaces for Clean and Energy-Efficient Diesel and Gasoline Power Trains European Commission
- Asst. Prof. Matej Andrej Komelj
- 7. FP MACAN; Merging Atomistic and Continuum Analysis of Nanometer Length-scale Metal-oxide Systems for Energy and Catalysis Applications European Commission
- Asst. Prof. Aleksander Rečnik
- 7. FP ESTEEM 2; Enabling Science and Technology through European Electron 9. Microscopy
- European Commission
- Prof. Miran Čeh
- 10. FP EURATOM; Development of Dense Beta SIC Matrix in 3D Preform 4.1.1.2.-FU; Annex 2 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Asst. Prof. Saša Novak Krmpotič
- 11. Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN-FUSEX
- Ministry of Higher Education, Science and Technology Asst Prof Saša Novak Krmpotič
- 12. 7. FP EURATOM, MHEST Association; Development of Dense Beta-SiC Matrix in 3D Preform - 4.1.1.2. - FU
- Ministry of Education, Science and Sport Asst. Prof. Saša Novak Krmpotič
- 7. FP EURATOM, MHEST Association; Development of Beta-SiC Fibres with W-CORE SiC Functional Materials 4.1.1.1. FU Ministry of Education, Science and Sport
- Asst. Prof. Goran Dražić
- 14. COST MP1005, NAMABIO; From Nano to Macro Biomaterials (Design, Processing, Characterization, Modelling) and Applications to Stem Cells Regenerative Orthopedic and Dental Medicine
- COST Office Asst. Prof. Saša Novak Krmpotič
- 15. MODEF Creazione e sperimentazione congiunta di modelli per l"ottimizzazione dell"utilizzo di energia fotovoltaica Unindustria Rovigo
 - Dr. Zoran Samardžija
- 16. Electron Energy-Loss Spectroscopy of Boron Incorporation in Strontion Aluminate Slovenian Research Agency
- Asst. Prof. Sašo Šturm 17. Minerals as a Precursors for Advanced Technologies
- Slovenian Research Agency Asst. Prof. Nina Daneu
- 18. Microstructural Investigation of Materials for Hydrogen Storage and Correlation with **Desorption Properties** Slovenian Research Agency Asst. Prof. Sašo Šturm
- VISITORS FROM ABROAD
- 1. Prof. Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 17.-22. 2. 2012 Prof. Michael Gasik, Aalto University School of Science and Technology, Faculty of
- Chemistry and Materials Science and Engineering, Espoo, Finland, 15.-17. 4. 2012 Süleyman Kahraman, M.Sc., Mustafa Kemal University, Physics Department, Hatay, 3. Turkey, 29. 3.-1. 9. 2012

- 19. Experimental and Theoretical Investigation of Hydrogen Sorption in Mg-Zr-Fe-Ni and Ti-Fe-Ni Systems Slovenian Research Agency
- Dr. Andraž Kocjan 20. NSFM: Novel Smart Filtration Media Dr. Kristina Žužek Rožman

RESEARCH PROGRAM

Nanostructured Materials Prof. Spomenka Kobe

R & D GRANTS AND CONTRACTS

- New metallic materials for thermal storage of digital information
- Dr. Andraž Kocjan
- Near-net shape nanoparticle-reinforced polymer-composites for highly-loaded advanced 2. mechanical components with superior tribological performance Asst. Prof. Saša Novak Krmpotič
- Novel functionalized nanomaterials for applications as nano- or biosensors/actuators/ bioresponsive (carrier) systems
- Dr. Kristina Žužek Rožman Twinning, epitaxy and phase transformations in minerals Asst. Prof. Nina Daneu
- Electron microscopy and microanalysis of materials on submicrometer scale 5 Dr. Zoran Samardžija
- 6. Hydrothermal synthesis of strongly adhered TiO2 photocatalytic coatings on metallic substrates Asst. Prof. Goran Dražić
- Microbial adhesion management on material surfaces 7. Asst. Prof. Goran Dražić
- Development of the model of the system for intelligent support of the selection of suitable powder material when developing sintered products
- Asst, Prof. Saša Novak Krmpotič Modification of TiO2 nanoparticle surface: prevention of agglomeration and 0 preservation of intrinsic properties Asst. Prof. Aleksander Rečnik
- 10. Innovative production systems for vaccines and regenerative medicine Asst. Prof. Aleksander Rečnik
- 11 Exploration and preservation of mineralogical heritage Asst. Prof. Aleksander Rečnik
- 12. High-coercivity Nd-Fe-B bonded magnets for automotive applications Prof. Spomenka Kobe
- 13. Protected Permanent Magnets for Advanced High-Temperature Applications Asst. Prof. Paul John Mcguiness
- 14. Materials and technologies for applications of ZnO-based thick-film varistors and oxide thermoelectrics Asst. Prof. Slavko Bernik
- 15. Colour, absorption and protective nanolayer coatings for aluminium alloy Prof. Miran Čeh

NEW CONTRACTS

- Cofinancing of the L2-4097 application project: High-coercivity Nd-Fe-B bonded magnets for automotive applications Kolektor Group, d. o. o.
 - Prof. Spomenka Kobe
- Cofinancing of the L2-4192 application project: Materials and technologies for applications of ZnO-based thick film varistors and oxide thermoelectrics Varsi, d. o. o. and Kekon, d.o.o. Asst. Prof. Slavko Bernik
- Cofinancing the L2-4099 application project: Protected permanent magnets for advanced high-temperature applications Magneti Liubliana, d. d.

Asst. Prof. Paul John McGuiness

- Prof. Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 26. 4. 2012
- Prof. Aldo R. Boccaccini, Universität Erlangen, Erlangen, Germany, 6.-11. 5. 2012
- Prof. Hans Jorg Meisel, BG Clinic Bergmannstrost, Department of Neurosurgery, Halle, 6. Germany, 27.-29. 5. 2012
- Prof. Mauro Alini, AO Research Institute, Davos Platz, Switzerland, 27.-29. 5. 2012 7.



- Prof. Thimios Mitsiadis, University of Zürich, Institute of Oral Biology, Zürich, 8 Switzerland, 27.-29, 5, 2012
- Prof. Andras Dinnyes, BioTalentum Ltd., Godollo, Hungary, 27.-29. 5. 2012
- 10. Prof. Dinko Mitrečič, School of Medicine, University of Zagreb, Zagreb, Croatia, 27-29 5 2012
- 11. Prof. Adrian Manescu, Università Politecnica delle Marche, Dip. DISCO, Ancona, Italy, 27.-29. 5. 2012
- 12. Prof. Nenad Filipovič, University of Kragujevac, Kragujevac, Serbia, 27.-29. 5. 2012
- 13. Prof. Petros Koidis, Aristotle University of Thessaloniki, School of Dentistry, Solun, Greece, 27.-29. 5. 2012
- Prof. Vitor Corello, Department of Polymer Engineering, University of Minho, Caldas das Taipas, Guimarães, Portugal, 27.-29. 5. 2012 15.
- Prof. Janis Locs, Riga Technical University, Riga Biomaterials Innovation and Development Centre Leading Researcher, Riga, Latvia, 27.-29. 5. 2012 Prof. Robert Zorec, Laboratory of Neuroendocrinology - Molecular Cell Physiology,
- Medical Faculty, University of Ljubljana, Ljubljana, Slovenia, 27.-29. 5. 2012 17. Asst. Prof. Mehmet Ali Gülgün, Melike Mercan Yildizhan, Sabanci University, Istanbul,
- Turkey, 27. 5.-3. 6. 2012 Asst. Prof. Cleva Ow-Yang, Faculty of Engineering and Natural Sciences, Sabanci
- University, 27. 5.-3. 6. 2012, 24. 10. 2012, 19.-23. 12. 2012
- 19. Dr. Goran and Dr. Zorica Branković, Institute for Multidisciplinary Research, Belgrade, Serbia, 19.-27. 8. 2012
- Hattori Yuto, Tokyo Institute of Technology, Tokyo, Japan, 29. 9. 2012–1. 3. 2013
 Dr. Jelena Pantić, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 9.–14. 9. 2012
- 22. Dr. Aleksandar Devečerski, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 9.-14.9.2012
- 23. Dr. Branko Matović, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 9.-14. 9. 2012
- 24. Prof. A. C. Cefalas, National Helenic Research Foundation NHRF, Athens, Greece, 22.-25.10.2012
- 25. Prof. Dragica Stojić, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 23.-26. 9. 2012
- 26. Katarina Čirić, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 23.-26. 9. 2012
- 27. Jana Radaković, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 23.-26. 9. 2012
- 28 Dr. Nikola Novaković, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 29. 10.-4.11.2012

- 29. Dr. Jasmina Grbović Novaković, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 29 10 -4 11 2012
- 30. Dr. Ljiljana Matović, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 29. 10.-4. 11. 2012
- Sandra Kurko, M.Sc., Vinča Institute of Nuclear Sciences, Beograd, Serbia, 29. 10.–4. 11. 2012
 Dr. Branislav Zlatkov, Volkswagen, Wolfsburg, Germany, 5. 10. 2012
- Dr. Wolfgang Kochanek, Kochanek Entwicklungsgesellschaft, Neustadt, Germany, 5. 10. 2012 33.
- 34. Dr Zoran Djinovic, Austrian Center for Medical Innovation and Technology, Wiener Neustadt, Austria, 5. 10. 2012
- 35 Prof. Rok Romih, Institute of Cell Biology, Medical Faculty, University of Ljubljana, Ljubljana, Slovenia, 24. 10. 2012
- 36 Dr. Olga Kazakova, National Physical Laboratory, Teddington, United Kingdom, 24. 10. 2012 Dr. César de Julián Fernández, CNR - Institute of Molecular Science and Technologies 37. (ISTM), Sesto Fiorentino, Italy, 24. 10. 2012
- 38 Prof. Josef Vleugels, Katholieke Universiteit Leuven, Leuven, Belgium, 20. 12. 2012
- 39. Asst. Prof. Mehmet Ali Gülgün, Sabanci University, Istanbul, Turkey, 19.-23. 12. 2012
- 40. Dr. Anne de Baas, European Coimmission, Brussels, Belgium, 19.-20. 12. 2012
- 41. Prof. Oliver Gutfleisch, Technische Universität Darmstadt, Darmstadt, Germany, 19.-20.12.2012
- 42. Dr. Nora Dempsey, Institut Néel CNRS/UJF, Grenoble, France, 19.-20. 12. 2012
- 43. Damien Le Roy, Institut Néel CNRS/UJF, Grenoble, France, 19.-20. 12. 2012
- 44. Dr. Thomas Schrefl, Fachochschule St. Pölten, St. Pölten, Austria, 19.-20. 12. 2012
- 45. Prof. Stefano Sanvito, Trinity College Dublin, Dublin, Ireland, 19.-20. 12. 2012
- Prof. Josef Fidler, Technische University of Wien, Wien, Austria, 19.-20. 12. 2012
- Dr. Boris Saje, Kolektor Group, d.o.o., Idrija, Slovenia, 19.-20. 12. 2012 47.
- Dr. Manfred Rührig, Siemens, Erlangen, Germany, 19.-20. 12. 2012
- 49. Kaan Üstüner M.Sc., Vacuumschmelze GmbH & Co., Hanau, Germany, 19.-20. 12. 2012
- 50. Dr. Jean-Marc Dubus, Valeo, Creteil, France, 19.-20. 12. 2012
- 51. Dr. Florian Lampmann, Daimler AG, Ulm, Germany, 19.-20. 12. 2012
- 52. Annemarie Gemperli, TEMAS AG, Arbon, Switzerland, 19.-20. 12. 2012
- 53. Dr. Jürgen Höck, TEMAS AG, Arbon, Switzerland, 19.-20. 12. 2012
- Dr. Thomas Woodcock, Leibniz-Institut für Festkörper- und Werkstoffforschung 54. Dresden, Dresden, Germany, 19.-20. 12. 2012
- Dr. Nikola Novaković, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 17.-21. 12. 2012 55
- 56. Dr. Ljiljana Matović, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 17.-21. 12. 2012
- 57. Adjelka Djukić, Vinča Institute of Nuclear Sciences, Beograd, Serbia, 17.-21. 12. 2012

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- Prof. Spomenka Kobe, Head 5.
- Asst. Prof. Matej Andrej Komelj 6.
- Asst. Prof. Paul John Mcguiness
- 8. Asst. Prof. Saša Novak Krmpotič
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- 11. Asst. Prof. Sašo Šturm
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- Postgraduates

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- Muhammad Shahid Arshad, M. Sc.
- 17. 18. Sandra Drev. B. Sc.
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- 20. Ana Gantar, B. Sc.

- 21. Barbara Horvat, B. Sc.
- 22. Aljaž Iveković, B. Sc.
- 23. Marja Jerič, B. Sc.
- 24. Nina Kostevšek, B. Sc. 25. Mateja Košir, B. Sc.
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- 28. Martina Lorenzetti, M. Sc.
- 29. Darja Pečko, B. Sc.
- 30. Matejka Podlogar, B. Sc.
- 31. Mojca Presečnik, B. Sc
- 32. Dr. Katarina Rade, left 01.06.12
- 33. Rok Rudež, B. Sc.
- 34. Marko Soderžnik, B. Sc
- 35. David Sojer, B. Sc.*
- 36. Nadežda Stanković, B. Sc.
- Janez Zavašnik, B. Sc. 37.

Technical officers

- 38. Sania Fidler, B. Sc.
- 39. Medeja Gec, B. Sc.

** postgraduate financed by industry

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ORIGINAL SCIENTIFIC ARTICLE

- Marcela Achimovičová, Francisco Jose Gotor, Concepcion Real, Nina Daneu, "Mechanochemical synthesis and characterization of nanocrystalline BiSe, Bi₂Se₃ semiconductors", *J. mater. sci., Mater. electron.*, vol. 23, no. 10, pp. 1844-1850, 2012.
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- 9. Maja Buljan, Nataša Radić, Sigrid Bernstorff, Goran Dražić, Iva Bogdanović-Radović, Václav Holý, "Grazing-incidence small-angle Xray scattering: application to the study of quantum dot lattices", *Acta crystallogr., A Found. crystallogr.*, vol. 68, no. 1, pp. 124-138, 2012.
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DEPARTMENT FOR MATERIALS SYNTHESIS

K-8

The research of the Department for Materials Synthesis is mainly related to the synthesis of different advanced materials, especially magnetic and semiconducting oxides. Special attention is given to nanostructured materials, such as ferrofluids, functionalized nanoparticles for use in biomedicine, multifunctional nanocomposites, and magnetic coatings for use in the microwave frequency range.

In 2012 our investigations have focused on three important materials, i.e., materials containing magnetic nanoparticles, microwave magnetic ceramic coatings for use in telecommunications, and ferroelectric materials with a high Curie temperature for the preparation of high-temperature, lead-free thermistors.

The research on magnetic nanoparticles has mainly been focused on magnetic carriers for applications in magnetic separation in biotechnology and medicine. Simple magnetic iron oxide is used as the material for the magnetic carriers, which have to be composed of magnetic nanoparticles that are small enough to be in the superparamagnetic state; that is below approximately 15 nm. Individual superparamagnetic nanoparticles are usually not efficient in magnetic separation, because of a too small magnetic force acting on them in a magnetic field gradient, which is the result of their very small volume. For an improved ability of magnetic separation, the superparamagnetic nanoparticles have to be agglomerated into nanoclusters, optimally with a size from 50 to 100 nm. The superparamagnetic nanoclusters were synthesized in the suspensions of superparamagnetic iron-oxide nanoparticles using two approaches. The first approach is based on the hetero-agglomeration (self-assembly)

of the nanoparticles in the suspensions. The driving force is the attractive electrostatic force between nanoparticles with an opposite surface charge or the chemical reactions between surface molecules. For the synthesis of the nanoclusters, the maghemite nanoparticles were coated with a thin layer of silica and grafted by silane molecules with either terminal amino groups (for a positive surface charge in aqueous suspensions), or with terminal carboxyl groups (a negative surface charge). For an easier analysis, one type of the nanoparticles was changed with equally functionalized silica nanoparticles.

The hetero-agglomeration of the two types of nanoparticles caused by the electrostatic interactions or by the chemical reactions between the surface amino groups and activated carboxyl groups has been systematically studied. For the synthesis of larger amounts of nanoclusters an emulsion method appeared to be more suitable. The method is based on use of a ferrofluid, i.e., a stable hexane suspension of the superparamagnetic maghemite na-

neurou is based on dec of a terroritid, i.e., a stable flexate suspension of a noparticles hydrophobised with oleic acid. Using the appropriate surfactant, the emulsion of the ferrofluid in water is formed. After evaporation of the hexane, a stable aqueous suspension of the nanoclusters is formed. Finally, the nanoclusters are coated with a thin silica layer (Figure 1). In cooperation with colleagues from Institute of Mathematics, Physics and Mechanics, Ljubljana, and from Vinča Institute, Beograd, Serbia, the magnetic properties of the nanoclusters were studied with a special focus on magnetic interactions between the individual superparamagnetic nanoparticles constituting the nanocluster.

The research of the magnetic nanoparticles for biomedical applications has mainly been focused on the synthesis of the maghemite nanoparticles coated with different biocompatible coatings. Currently, only maghemite nanoparticles coated with dextran or its derivate carboxymethyl dextran (CMD) are actually used for *in-vivo* applications. The biocompatible polysaccharide coating enables the colloidal stability of the nanoparticles in physiological fluids. The coated nanoparticles can be synthesized either in a two-step procedure, including coating of the previously synthesized

nanoparticles with the polysaccharide, or in a one-step procedure based on synthesizing the nanoparticles using the co-precipitation of the Fe ions from the aqueous solutions in the presence of the polysaccharide. In the latter case, the mechanism of the nanoparticle formation is significantly changed. The formation of the maghemite nanoparticles during co-precipitation in the presence of CMD has been systematically studied in a cooperation

Hetero-agglomeration of nanoparticles in their aqueous suspensions based on electrostatic interactions between the nanoparticles displaying the opposite surface charge or based on chemical reactions between molecules on their surfaces.



Figure 1: TEM image of superparamagnetic nanoclusters coated with a thin silica layer.



with the pharmaceutical company Lek d.d.. It appeared that the process of the nanoparticle formation is decisively influenced by the formation of a Fe³⁺-CMD complex prior to the precipitation of the ions. The bonding of different amino acids onto the maghemite nanoparticles with subsequent adsorption or during their synthesis in the presence of the amino acid has also been studied.

We also cooperated in nanotoxicology research with the Biotechnical Faculty, University of Ljubljana, where we provided our expertise in the synthesis, functionalization and characterization of nanoparticles.

The synthesis of cobalt-ferrite nanoparticles ($CoFe_2O_4$) and their stable suspensions was also investigated. We focused on spinel ferrite nanoparticles in the size region from sizes where superparamagnetism dominates to the region where ferrimagnetism dominates the magnetic properties. For certain applications, colloidal suspensions of ferrimagnetic nanoparticles in various carrier liquids are desired. The preparation of the suspensions and their colloidal and magnetic properties have been systematically studied. Oleic acid was used as the surfactant for the nonpolar media and citric acid for the aqueous media.

 $CoFe_2O_4$ shows magnetic properties that are not typical for spinel ferrites, i.e., a high magnetic anisotropy, which results in high coercivity and magnetostriction. It shows the largest magnetostriction among oxide materials

A procedure for the synthesis of superparamagnetic nanoclusters for applications in magnetic separation was developed. and is therefore suitable for applications in multifunctional composites like: magneto-dielectrics, in which magnetic and dielectric (ferroelectric) properties are mechanically coupled. The properties of such composites depend on the basic properties of the constituent phases and on the specific phase distribution in the material. We studied the effect of colloidal and magnetic

properties of CoFe_2O_4 nanoparticles, dispersed in water, on the assembly of CoFe_2O_4 nanoparticles into columnar structures under an applied magnetic field (Figure 2). We showed that the shape and density of the columnar structures strongly depend on the magnetic interactions between the CoFe_2O_4 nanoparticles determined with the



Figure 2: Columnar magnetic structures prepared using the directed assembly of cobalt-ferrite nanoparticles in a magnetic field.

strength of the applied magnetic field and the particles' magnetic properties. Such structured deposits can be further used as a basis for the fabrication of magneto-dielectrics with the 1-3 structure type, which are supposed to show the largest coupling between the two phases. BaTiO₃ and Pb(Zr,Ti) O₃ (PZT) were the selected dielectric phases. We studied their chemical compatibility with CoFe₂O₄ during the co-sintering of the two functional phases. Although we could not completely prevent the interdifussion of small cations (in particular Fe³⁺ and Ti⁴⁺) below 1000°C, we managed to tune the sintering behaviour of CoFe₂O₄ and PZT by pre-firing the CoFe₂O₄ nanoparticles at 700°C. In such a way, we managed to prevent cracking at the interfaces during the co-sintering at 950°C.

Our research in cooperation with researchers from the Faculty of Mathematics and Physics, University of Ljubljana was also related to nanomaterials synthesis in suspensions. Incorporation of superparamagnetic nanoparticles into polydimethylsilixane (PDMS) polymer was investigated for applications in photolithography and microfluidics. We have developed a procedure for the functionalization of silica-coated magnetic nanoparticles with modified PDMS providing a homogeneous distribution of magnetic nanoparticles inside the final elastomer.

The synthesis of thin amorphous silica shells on the surfaces of liquid-crystal droplets was studied in cooperation with our colleagues from Department for Condensed Matter Physics, JSI. The materials could find applications in photonics. For this purpose the most suitable surfactants were prepared, providing good colloidal stability of the liquid-crystal droplets in water. The liquid-crystal droplets were then coated with a thin silica shell using hydrolysis and the polycondensation of tetraethyl orthosilicate (TEOS) in alkaline conditions.

A part of our research was also devoted to the synthesis of other magnetic materials, in particular those with a crystallization that requires high temperature. Hydrothermal synthesis is normally used in such cases. We

Mechanisms of maghemite nanoparticles' formation during the precipitation of iron ions in the presence of carboxymethyl dextran or different amino acids. have focused on the hydrothermal synthesis is normally used in other cases. we have focused on the hydrothermal synthesis of dendrites of the magnetic perovskite $LaSrMnO_3(LSMO)$ and of nanoparticles of spinel ferrite Mg(Ti) Fe_2O_4 . The Curie temperature of both materials can be tuned by changing their composition to values that enable applications in cancer treatment using self-regulating magnetic hyperthermia. In the synthesis of LSMO we focused on the research of mechanisms leading to dendrite formation. A

new mechanism for dendrite nucleation was proposed. During hydrothermal treatment at lower temperatures hexagonal platelet crystals of a SrMnO₃-La solid solution with a hexagonal perovskite structure form first. At higher temperatures the LSMO perovskite nucleates epitaxially at the edges of the hexagonal crystal and grows outwards,

forming the dendrite structure (Figure 3). With a further increase in the temperature this causes further growth of the structure into dendrites of a hexagonal "snowflake" shape or the dendrites break from the template and form a structure with a specific shape of "pine trees".

A large part of our research was devoted to the synthesis and detailed characterisation of nanocomposite particles synthesized using a coating of thin layers of magnetic iron oxide onto different core nanoparticles using

simple precipitation from aqueous solutions. We have focused on nanocomposite particles composed of a hard-magnetic hexaferrite core and a soft-magnetic maghemite shell deposited using the procedures developed in previous years. Such nanocomposite particles would display an optimal shape of their magnetic hysteresis for use in magnetic hyperthermia. Highresolution electron microscopy showed that the maghemite grew epitaxially

Synthesis, structure and magnetic properties of nanocomposite particles composed of a hardmagnetic hexaferrite core and the soft-magnetic maghemite shell.

on the structurally similar hexaferrite core with spinel {111} planes parallel to the hexaferrite basal {0001} planes (Figure 4). A lot of attention was given to a study of the magnetic coupling between the two phases. The main focus

on the synthesis of the nanocomposite particles part has been given to the research of a procedure appropriate for coating hard-magnetic cobalt ferrite onto different core nanoparticles.

We continued our research on the synthesis of nanocomposite particles used for the decomposition of organic pollutants in water. The nanocomposite particles are composed of photocatalytic anatase (TiO₂) nanoparticles coated onto agglomerates of superparamagnetic maghemite (Fe₂O₂) nanoparticles. For the photocatalytic purification, the particles are dispersed in polluted water. The surface anatase layer provides a high photocatalytic activity, while the superparamagnetic cores enable the separation of the particles from the suspension after the purification and their re-use. Besides the applied research financed by the company Cinkarne Celje, which was mainly devoted to the development of procedures for the industrial production of materials, the basic research was also conducted. This research was manly oriented to mechanisms enabling an increase in the photocatalytic activity of the materials using the doping of anatase. The incorporation of an acceptor dopant Fe³⁺ and a donor dopant W⁶⁺ into the anatase structure of the nanoparticles during their synthesis using co-precipitation from aqueous solutions or the hydrothermal method were studied.

The studies in the field of magnetic materials for telecommunications were focused on the development of ceramic films for micro- and mm-wave applications. Our aim was to develop a simple method for the preparation of magnetically-oriented thick hexaferrite films with low magnetic losses that

are suitable for self-biased nonreciprocal devices, operating at mm-waves. Two parallel studies were conducted: electrophoretic deposition (EPD) and deposition in a magnetic field. We explained the mechanism for the orientation of particles during the EPD based on the effect of electrophoretic and hydrodynamic forces acting on thin plates during the EPD. The plates move towards the oppositely charged electrode due to the electrophoretic force. Their movement is opposed by a hydrodynamic friction, which preferentially orients the plates perpendicular to the electrode (i.e., substrate). The direction of the hydrodynamic flow changes in the vicinity of an electrode and, consequently, the plates reorient in parallel with the electrode. We confirmed our experimental results from previous years with

theoretical calculations. Specifically, we confirmed that the alignment degree of the deposits increases with the increasing shape anisotropy of the hexaferrite particles, with increasing stability of suspensions and at lower electric field, i.e., with slower EPD kinetics. We managed to prepare $BaFe_{12}O_{19}$ films with around 90% magnetic orientation and a thickness up to 30 mm based on the optimized particle-size distribution and EPD parameters followed by sintering at 1150°C. These films are suitable for self-biased applications.

The magnetic properties of the cobalt-ferrite nanoparticles critically influence the formation of columnar structures during the process of the magnetically-directed assembly of colloidal nanoparticles.

In parallel, the magnetically directed assembly of $BaFe_{12}O_{19}$ particles was studied. This approach did not result in a significant improvement of the magnetic orientation of films in comparison to EPD. However, it is more suitable for high-frequency applications, for which the magnetic layer should be isolating. Namely, the EPD is based on a conductive substrate. Theoretical calculations were also applied within this study to evaluate and support the experimental evidence. We showed that large $BaFe_{12}O_{19}$ plates (with diameters of few 100 nm) possessing significant magnetic moment agglomerate when they are exposed to magnetic field, thus reducing the expected magnetic alignment. In contrast, very small plates (with diameters of up to 10 nm) are not significantly affected by the ap-



Figure 3: Growth of magnetic perovskite LaSrMnO3 dendrites from a SrMnO3 crystal displaying a hexagonal-perovskite structure.

plied magnetic field and their magnetic alignment is therefore limited. The optimal alignment of $BaFe_{12}O_{19}$ plates can be achieved using a combination of small plates with a minor concentration of larger ones. Here, the large

Influence of materials and processing parameters on the directed assembly of barium-hexaferrite nanoparticles in electric and magnetic fields. of small plates with a minor concentration of larger ones. Here, the large plates direct the alignment of the smaller ones. Thus we prepared $BaFe_{12}O_{19}$ films with a magnetic orientation above 90% under a magnetic field of 0.02 T and with sintering at 1150°C.

The studies described above served as a basis in the realisation of an international applicative project FERFIT under the coordination of K8. The project finished at the end of 2012. The aim of the project was to develop unnetically oriented films based on BaFe O. Such films can be applied as self.

methods for the preparation of magnetically oriented films based on $BaFe_{12}O_{19}$. Such films can be applied as self-biased nonreciprocal devices. This year we have intensively studied EPD using a degradable electrode-substrate and



Figure 4: Nanocomposite particles composed of a hard-magnetic hexaferrite (HF) core and the soft-magnetic spinel (S) maghemite shell.

EPD in nonpolar media. In the latter case, we achieved magnetic orientation of the films above 90% due to slow EPD kinetics. Within the same project we have also been involved in the optimization of the screen-printing parameters of $BaFe_{12}O_{19}$ thick films, for which a magnetic field of 24 Moe was applied during their drying to induce the magnetic alignment. Chemically modified $BaFe_{12}O_{19}$ films with thicknesses of around 80 mm were used for the construction of a pilot circulator operating at 30-40 GHz.

This year we also upgraded the previous studies related to the partial substitution of Fe^{3+} in $BaM_xFe_{12-x}O_{19}$ (M = In, Cr) from the FERFIT project to more basic ones. We studied the mechanisms of the substituent effect on the particle size during hydrothermal synthesis. Namely, already a minor substitution of In^{3+} significantly changes the particle-size distribution, which was not observed for the substitution with Cr^{3+} . We showed that the kinetics of nucleation and particle growth can be influenced only by M^{3+} larger

than Fe³⁺ (besides In³⁺ also Sc³⁺). In this way, we solved the problem of exaggerated BaFe₁₂O₁₉ particle growth at a high enough hydrothermal synthesis temperature that allows the synthesis of well-crystallized nanoplates of BaM_xFe_{12-x}O₁₉ (M = In, Sc) with applicable magnetic properties. These nanoparticles were dispersed in 1-butanol and incorporated by colleagues from the Department of Complex Matter (F7) into liquid crystals to induce specific ferromagnetic ordering due to the particles' shape anisotropy.

We were involved in the development of magnetically oriented thick barium-hexaferrite films that were integrated into a self-biased mmwave circulator. In the field of high-temperature thermistors the processes of reduction and re-oxidation related to the formation of temperature-dependent potential barriers at the grain boundaries of ferroelectric ceramics in the systems BaTiO₃-Na_{0.5}Bi_{0.5}TiO₃. In this system, the PTC resistors displaying Curie temperature of 180 °C and low room-temperature specific resistivity were developed.

Some outstanding publications in the past year

- 1. Kralj, S., Rojnik, M., Romih, R., Jagodič, M., Kos, J., Makovec, D.: Effect of surface charge on the cellular uptake of fluorescent magnetic nanoparticles. J. nanopart. res., 2012, vol. 14, no. 10, 1151-1-1151-14
- Lisjak, D., Drofenik, M.: Chemical substitution an alternative strategy for controlling the particle size of barium ferrite. Cryst. growth des., 2012, vol. 12, no. 11, pp. 5174–5179
- 3. Lisjak, D., Ovtar, S.: The alignment of barium ferrite nanoparticles from their suspensions in electric and magnetic fields. J. phys. chem., B Condens. mater. surf. interfaces biophys., [in press], 2012, p. 7

Patent granted

 Marin Berovič, Darko Makovec, Suzana Bošković, Process of magnetic precipitation of yeast biomass from sparkling wine, SI23583 (A), Urad RS za intelektualno lastnino, 29.6.2012

INTERNATIONAL PROJECTS

- COST MP0701; Composites with Novel functional and structural properties by nanoscale materials (Nano Composite Materials NCM) COST Office
- Prof. Darko Makovec
- Room-temperature multiferroics based on Y-type hexaferrites Slovenian Research Agency Asst. Prof. Darja Lisjak

RESEARCH PROGRAM

1. Advanced inorganic magnetic and semiconducting materials Prof. Darko Makovec

R & D GRANTS AND CONTRACTS

1. FERFIT: Ferrite thick films for integrated circuits Asst. Prof. Darja Lisjak

NEW CONTRACT

1. Optimization of iron oxide nanoparticles synthesis - analytical and expert support Lek d d Prof. Darko Makovec

VISITORS FROM ABROAD

- 1. Svetoslava Mihaylov Kolev, Institute of Electronics, Bulgarian Academy of Sciences, 1.-31.8.2012
- 2. Dr. Marin Tadič, Vinca Institute, Condensed Matter Physics Laboratory, University of Belgrade, Belgrade, Serbia, 1. 9.-1. 12. 2012

STAFF

Researchers

- Prof. Mihael Drofenik*, retired 30.12.12
- Asst. Prof. Darja Lisjak Prof. Darko Makovec, Head
- 3.

4. Dr. Igor Zajc Postdoctorial associates

- 5. Dr. Sašo Gyergyek
- 6. Dr. Slavko Kralj
- Asst. Prof. Matjaž Kristl*
- Dr. Simona Ovtar, left 01.08.12
- Postgraduates
- 9. Peter Dušak, B. Sc.

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- 11. Olivija Plohl, B. Sc.
- 12. Darinka Primc, B. Sc.
- 13. Klementina Pušnik, B. Sc.
- 14. Aljaž Selišnik**

Technical and administrative staff 15. Bernarda Anželak, B. Sc.

Note:

- * part-time JSI member ** postgraduate financed by industry
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PATENT

1. Marin Berovič, Darko Makovec, Suzana Bošković, *Process of magnetic precipitation of yeast biomass from sparkling wine*, SI23583 (A), Urad RS za intelektualno lastnino, 29.6.2012.

MENTORING

- 1. Brina Dojer, *The comparison of structural and magnetic properties of cobalt(II) and nickel(II) acetates with N-donor ligands:* doctoral dissertation, Maribor, 2012 (mentor Mihael Drofenik; co-mentor Matjaž Kristl).
- Ana Drmota Petrič, Synthesis and characterization of magnetic nanoparticles for electromagnetic wave absorbers: doctoral dissertation, Maribor, 2012 (mentor Mihael Drofenik).
- Slavko Kralj, Functionalization of magnetic nanoparticles for biomedical applications: doctoral dissertation, Ljubljana, 2012 (mentor Darko Makovec; co-mentor Janko Kos).
- 4. Simona Ovtar, *Magnetically oriented films of barium ferrite:* doctoral dissertation, Ljubljana, 2012 (mentor Darja Lisjak).

DEPARTMENT FOR ADVANCED MATERIALS

The main activities of the department encompass basic and applied research within the fields of energy materials, biomaterials and electronic materials. Among the important objectives are the development of new, efficient oxides for high-temperature thermoelectric energy conversion, materials with improved antibacterial and photocatalytic effects and the development of thin films and nanostructured powders of functional electronic oxides for various applications.

Thermoelectric oxides

The research of oxides as possible thermoelectric materials was triggered by the discovery that metallic layered cobaltate Na_CoO₂ exhibits a large Seebeck coefficient combined with a high electrical conductivity and a low thermal conductivity, which was attributed to its layered crystal structure consisting of two-dimensional sheets of edge-sharing CoO₆ octahedra intercalated by Na ions. The highest reported zT values of Na_xCoO₂ are ~1.0 for singlecrystalline and ~ 0.8 for polycrystalline material at temperatures in the vicinity of 800°C. With such properties it was considered to be a good candidate for the high-temperature p-type thermoelectric material. However, the chemistry Head: of layered sodium cobaltates is governed by the high mobility of interlayer sodium, which reacts with atmospheric Prof. Danilo Suvorov moisture and carbon dioxide. Furthermore, the layered crystal structure of Na Co O, enables the intercalation of molecules such as water, which can lead to exfoliation and thus degradation of the material. Because of this the focus of the research turned to a semiconducting misfit-layered cobaltate Ca₂Co₄O₆, the structure of which consists

K-9

of triple Ca₂CoO₂ layers and single layers of CoO₂ analogous to CoO₂ sheets of Na CoO₂ compounds. The highest zT reported for this structural type was \sim 0.6. We found that the sheets of octahedrally coordinated Co ions, which are the common structural element of the Na COO, and Ca CO O, phases, allow the spontaneous intergrowth of the two structures (Fig. 1) leading to a significant improvement of environmental stability. Furthermore, the coherent intergrowth of the two structural types results in effective texturing in polycrystalline material with the preferred grain growth aligned in-plane with common CoO_c layers, thus allowing high electrical conductivity. The nanostructured intergrowths also result in a significant reduction of the thermal conductivity, which was at 700°C measured to be ~ 0.3 W/mK for the "out-of plane" and ~ 0.6 W/mK for the "in-plane" direction. With the measured power factor of $\sim 6.5*10^4$ W/mK² the calculated "in-plane" zT of the intergrowth structure material with the nominal composition $Ca_2 Na_0 Co_4 O_0$ is ~1.0 at 700°C, which is higher than any so-far reported value for oxide thermoelectrics.



An innovative concept has been applied to develop human and environmentally friendly material with antibacterial properties. The material is a composite formed of bioceramic, metallic and organic phases that contain amino and thiol groups. Metallic nanoparticles have a functionalized surface and they are carriers of antibacterial activity. The efficacy of the antibacterial action of the composites depends on the type of surface functionalization that provides activity against Gram-positive and Gram-negative bacteria. The materials were prepared by a sonochemical method that was developed as a novel route for the synthesis of this type of material and belongs to green chemistry. The developed materials have a stronger antibacterial activity in comparison to silver-based materials that are frequently used in practice, which indicates the possibility of their replacement by novel, more effective and safer materials developed in our laboratory. The morphological properties of the newly developed material and its antibacterial activity are shown in Fig. 2.



Figure 1: HRTEM image and SAED pattern of coherently intergrown $Na_{x}CoO_{2}$ and $Ca_{3}Co_{4}O_{0}$ structure types.



Figure 2: Morphological properties of a novel antibacterial material and its antibacterial effect on E. coli, developed at the Advanced Materials Department.

In the field of photocatalytic materials, hierarchically assembled nanostructured spherical anatase particles in the size range from 3 to 7 mm, using a solvothermal synthesis method, were prepared. The spherical particles are composed of nanosized primary crystallites with a size below 30 nm. The prepared anatase exhibits good photocatalytic properties and a high temperature stability, over 1000°C. Due to the large particle size, these particles are less harmful, compared to nanosized commercial anatase.

Functional electronic oxides

In the scope of the European project "Nanostructured Ferroelectric Films for Biosensors" we studied the synthesis and characterization of $Pb(Mg_{1/3}/Nb_{2/3})O_3$ -PbTiO₃ thin films prepared on Pt(111)/TiO₂/SiO₂/Si substrates using the sol-gel method for Film Bulk Acoustic Resonator (FBAR) sensor applications. In order to determine the influence

In collaboration with Epcos OHG, a member of the TDK-EPC Corporation, we developed a p-type thermoelectric oxide with zT \sim 1.0 at 700°C, which makes it superior to so-far reported polycrystalline thermoelectric oxides. The invention is EU patent pending.

Resonator (FBAR) sensor applications. In order to determine the influence of the coordination chemistry on the formation of the perovskite the conditions of the reagents were systematically varied. As a source of Mg-precursor $Mg(CH_3COO)_2 \times 4H_2O$, $Mg(AcAc)_2 \times 2H_2O$ and $Mg(NO_3)_2 \times 6H_2O$ were applied to reduce the concentration of the undesired pyrochlore phase that forms in addition to the perovskite phase. $Pb(NO_3)_2$, $Pb(CH_3COO)_2$, $Pb(PVP)_2$ and $Pb(AcAc)_2$ were used as a source of Pb. Changing the coordination sphere of Mg does not increase the reactivity of Mg ions towards Nb to the point that they will preferentially react, forming the Mg-O-Nb heterometallic structure.

A pyrochlore-free $Pb(Mg_{1/3}/Nb_{2/3})O_3$ -PbTiO₃ film was formed when the steric hindrance of the Pb precursor was increased. In this way the reactivity of Pb ions towards Nb ions is decreased, resulting in the formation of Mg-O-Nb heterometallic clusters, leading to the formation of a perovskite phase. Thus, Pb(PVP)₂ and Pb(AcAc)₂ were shown to be effective in the formation of pyrochlore-free thin films.

It was observed that during the direct casting of the film on the $Pt(111)/TiO_2/SiO_2/Si$ substrate the films grow into a dense and crack-free microstructure. The relative permittivity and dielectric losses for the pyrochlore-free PMN-PT thin film were found to be 1650 and 0.12, respectively.

We further investigated the tunable properties of $(1-x)Na_{0.5}Bi_{0.5}TiO_3$ -xNaTaO₃ thin films (0.05<x<0.3) prepared by a modified sol-gel method. A dense and homogenous microstructure, with the average grain size ranging between 70 and 110 nm, was obtained for the NBT-NTa thin films by using a Bi-propionate precursor in the sol-gel synthesis. It was observed that the dielectric permittivity increases with the annealing temperature for all the prepared NBT-NTa thin-film compositions. The decrease in the average grain size below 150 nm caused the appearance of

In the scope of the Center of Excellence in Nanoscience and Nanotechnology we set up the first Pulsed Laser Deposition (PLD) laboratory in Slovenia dedicated to the layer-by-layer growth of inorganic thin films. single-domain grains, which then strongly affected the polarization behavior of the 5NTa thin films, giving them a relaxor-type response. The relaxor-type and paraelectric-type responses were observed for the 10NTa and 30NTa thin films, respectively. Comparable dielectric permittivity and relative tunability values were obtained for the 5NTa (e = 441, $n_r = 42\%$) and the 10NTa (e = 440, $n_r = 40\%$) thin films, whereas the 30NTa thin films showed lower values (e = 370, $n_r = 23\%$).

In the field of ferroelectric thin films, research is driven by demands to improve and tailor the inherent material's electrical response. The motivation behind our investigation was directed towards tuning the temperature-dependent dielectric behavior and improving the dielectric loss characteristics. In this attempt, we designed $SrTiO_3/Na_{0.5}Bi_{0.5}TiO_3/SrTiO_3$ (ST/NBT/ST) structured thin films, where the ferroelectric NBT phase is embedded within a low-dielectric-loss ST component. Using repeated thermal treatment we managed to prepare thin films with a temperature flat dielectric permittivity (te of 780 ppm/K in the temperature range between -50°C and 200°C), decreased dielectric losses, and a frequency undispersed response at room temperature. The obtained results were attributed to the compositional gradient between particulate ST and NBT layers, as determined by X-ray diffraction and X-ray photoelectron spectroscopy. As-structured thin films exhibit promising properties for functional devices that are required to produce stable performance in a broad temperature range.

Beyond sol-gel techniques we utilized diblock-copolymers (BCs) to synthesize multifunctional thin films. Due to the different chemical nature of the separate blocks they self-organize into different phases, where the type of the phase depends on the block fraction ratio, the monomer chemical nature, the temperature, etc. In our work we take advantage of a polystyrene-polyethylene oxide (PS-b-PEO) block-copolymer to obtain $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) / SrTiO_3 (ST) or Pb(Mg_{1/3}Nb_{2/3}O_3-PbTiO_3 (PMN-PT) / CoFe_2O_4 (CF) multifunctional thin films with in-plane interfaces. Using a different polarity of the precursors or specific casting procedures we can selectively direct inorganic components into the PS or PEO block. In the first part of the study we investigated the self-assembling properties of the BC solely. We observed that the morphology of the films is highly dependent on the casting conditions. Films cast under ambient conditions presented no preferential orientation. A short anneal in toluene vapor orients the PS-b-PEO into a hexagonal order. Subsequently, multifunctional thin films were prepared from the NBT and ST sols

or the PMN-PT sol and CF nanoparticles. Using the proper casting conditions and thermal treatment we managed to prepare films, for which grazing incidence X-ray diffraction confirmed the presence of NBT/ST or PMN-PT/CF. This is especially important for NBT/ST, since they easily form a solid solution across the entire compositional range.

Within the European project "Novel Inorganic Inks for Hybrid Printed Electronic Demonstrators" we investigated the synthesis of differently shaped ferroelectric particles. The experimental conditions for the growth of shape-controlled $BaTiO_2$ particles in NaOH and barium salt $(Ba(NO_2)_2)$ BaCl₂ or Ba(CH₂COO)₂) aqueous and water/ethanol solutions using various TiO₂-containing precursors (Ti-precursor) were studied. We found that different chemistries and physical characteristics of the Ti-precursors resulted in different BaTiO, formation rates, morphologies and phase compositions. Nanocrystalline anatase, TiO, aerogel and sodium titanates (NT) belts led to cubic BaTiO₂ at temperatures of 80-230°C, while tetragonal BaTiO₂ formed from potassium titanate (KT) at 150-230°C. The morphology of the BaTiO, prepared from KT at low temperatures (80-100°C), did not differ significantly from that obtained from NT belts and TiO, aerogel. These precursors, which reacted slowly in alkaline aqueous media, produced single-crystalline star-like particles. The fastest BaTiO, formation rate was observed for nanocrystal-



Figure 3: Pulsed laser deposition (PLD) system with laser and optical cahinet

line anatase, which led to irregularly shaped BaTiO, particles. According to TEM investigations, the growth of the single-crystalline star-like BaTiO, particles occurred via the oriented attachment of nanocrystals, which formed from the dissolved barium and titanium species. The modification of the water solution by the addition of ethanol or excess of NaOH caused the morphological change from star- to square-like particles, which similar to stars became irregularly shaped above 100°C. The modifications of the solution are believed to influence both the nucleation and aggregation process and consequently changed the particle shape from star- to square-like.

In the scope of the Center of Excellence in Nanoscience and Nanotechnology we set up the first Pulsed Laser Deposition (PLD) system in Slovenia, which is a powerful technique for the thin-film growth of inorganic materials (Fig. 3). The delivered system is dedicated for layer-by-layer growth and thus enables the preparation of high-quality thin films and structuring on a nanoscopic level. The system is equipped with the following major components: heater stage for laser and resistive heating of substrates, target scanning stage, loadlock for sample and target transfer, high-pressure reflection high-energy electron diffraction system, upgrade with UHV pumps (titanium sublimation pump, ion pump), oxygen plasma source, sputter source (1 x 1.3" target), connection with a glovebox. For the

ablation of the target material a KrF excimer laser is used with an energy up to 700 mJ per pulse and a maximum repetition rate of 50 Hz. The system is mainly utilized for the deposition of functional oxides on silicone substrates. Interfacing an oxide with silicon is a great challenge that has attracted a lot of interest in the industrial and scientific community so far. Solving the interface problem would enable the further scaling of microelectronic devices to smaller dimensions and the growth of high-quality oxides with different functionalities on a silicon platform, which can be exploited in micro-electro-mechanical systems, random-access memories, and other oxide-based nano-electronic devices. In our study, pulsed laser deposition (PLD) was used to study the interfaces between SrTiO₂ (STO) thin films and silicon. Before the deposition the native oxide on the silicon was removed by HF dip, while in order to understand the interfacial structure in more detail, we performed kinematical simulations of the reflection high-energy electron diffraction (RHEED) patterns. The RHEED patterns were calculated for unreconstructed and reconstructed Si(001) surface with up to four atomic layers and for each of these models we used two different azimuth directions, [100] and [110].

Using a HF treatment of silicon substrate we obtained H-terminated surface, which prevents silicon from oxidising. On such substrates STO was deposited directly or using SrO as a buffer layer. The results show that the optimum conditions involve a two-step procedure, in which the initial vacuum and the lower deposition temperature have an important role. In the case of the direct deposition of STO the obtained films are preferentially textured with a (100) orientation. The application of SrO enabled partially epitaxial growth of STO with STO(110) | |Si(100) and STO[100] | | Si[110] (Fig. 4). The change of the growth orientation induced by SrO was governed by the formation of the SrO(111) intermediate layer and subsequently Figure 4: HRTEM image of STO deposited on SrO-buffered Si by the minimization of the lattice misfit between the STO and SrO.



substrate.

Organization of conferences, congresses and meetings

- 1. Journal of European Ceramic Society Trust Meeting, Ljubljana, Slovenia, 2. 2. 2012.
- 2. Permanent Executive Committee of the European Ceramic Society Meeting, Ljubljana, Slovenia, 3. 2. 2012.
- 3. Materials, Science and Technology 2012 Conference and Exhibition, Pittsburgh, USA, 7.-11. 10. 2011, co-organizers
- 4. 20th Conference on Materials and Technologies, Portorož, Slovenia, 17.-19. 10. 2012, co-organizers

Patents granted

- 1. Aleš Dakskobler, Andraž Kocjan, Manca Logar, Method for the preparation of carrier colloidal powder with high specific surface area, SI23502 (A), Urad RS za intelektualno lastnino, 30.4.2012.
- 2. Aleš Dakskobler, Andraž Kocjan, Manca Logar, Method for the preparation of carrier colloidal powder with high specific surface area, SI23580 (A), Urad RS za intelektualno lastnino, 26.6.2012.

INTERNATIONAL PROJECTS

- 1. Thermoelectric oxide materials EPCOS OHG Ceramic Components Division Prof. Danilo Suvorov
- Microwave tunable materials, composites and devices NATO - North Atlantic Treaty Organisation Asst. Prof. Boštian Iančar
- The synthesis of dielectric materials by chemical solution deposition and characterization of their dielectric properties Slovenian Research Agency Prof. Danilo Suvorov
- Nanostructural designing of multifunctional and sintered electrical and biological functionally graded materials Slovenian Research Agency Asst. Prof. Srečo Davor Škapin

RESEARCH PROGRAM

1. Contemporary inorganic materials and nanotechnologies Prof. Danilo Suvorov

R & D GRANTS AND CONTRACTS

1. Nanoengineering of self-assembled materials Prof. Danilo Suvorov

VISITORS FROM ABROAD

- 1. Dr. Tim Jackson, School of Electronic, Electrical and Computing Engineering, University of Birmingham, Birmingham, Great Britain, 18.–20. 1. 2012
- Prof. Anatolii Bilous, Dr. Oleg Ovchar, Vernadskii Institute of General and Inorganic Chemistry, Ukrainian National Academy of Sciences, Kiev, Ukraine, 18.–20. 1. 2012
- 3. Prof. Ivan Sondi, University of Zagreb, Zagreb, Croatia, 24. 2. 2012
- Dr. Marija Vukomanović, Institute of Technical Sciences, Serbian Academy of Sciences and Arts, Belgrade, Serbia, 2.–6. 4. 2012
- Dr. Christoph Auer, Hermann Gruenbichler, Dr. Yongli Wang, TDK EPCOS, Deutschlandsberg, Austria, 14. 6. 2012
- Dr. Jae Ho Jeon, Korea Institute of Materials Science, Changwon, Korea, 20.–22. 6. 2012
 Prof. Dragoljub Uskoković, Institute of Technical Sciences, Serbian Academy of Sciences and Arts, Belgrade, Serbia, 21.–22. 6. 2012
- 8. Prof. Jose Varela, São Paulo State University, Araraguara, Brazil, 22. 6. 2012
- 9. Dr. Marcelo Orlandi, São Paulo State University, Araraquara, Brazil, 29. 6.-15. 7. 2012
- Dr. Smilja Marković, Institute of Technical Sciences, Serbian Academy of Sciences and Arts, Belgrade, Serbia, 23. 7.–3. 8. 2012
- Prof. Dragoljub Uskoković, Institute of Technical Sciences, Serbian Academy of Sciences and Arts, Belgrade, Serbia, 26.–27. 7. 2012

- Functionalization of the surface of organic pigments for durable, efficient and colourstable paints Asst. Prof. Srečo Davor Škapin
- Self-cleaning antibacterial fotocatalitic coatings in whitewear production Prof. Danilo Suvorov
- Physics and chemistry of porous aliminium for Al panels, capable of higly efficient energy absorbtion Prof. Danilo Suvorov
- New materials for power conversion: oxide semiconductor thermoelectrics Prof. Danilo Suvorov
- 6. INNOINKS: Novel inorganic inks for hybrid printed electronic demonstrators Prof. Danilo Suvorov
- NAFERBIO: Nanostructured ferroelectric films for biosensor Prof. Danilo Suvorov

NEW CONTRACTS

- New materials for energy conversion: oxide semiconducting thermoelectrics Gorenje Household Appliances, d. d. prof. dr. Danilo Suvorov
- Development and characterisation of mineral wool fibres Knauf Insulation, d. o. o. Prof. Danilo Suvorov

- 12. Dr. Dragana Jugović, Institute of Technical Sciences, Serbian Academy of Sciences and Arts, Belgrade, Serbia, 25. 10. 2012
- 13. Dr. Miodrag Mitrić, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 25. 10. 2012
- Dr. Jyoti Prosad Guha, Missoury University of Science and Technology, Rolla, ZDA, 9. 10.–15. 11. 2012
- Miodrag Lukić, Dr. Smilja Marković, Institute of Technical Sciences, Serbian Academy of Sciences and Arts, Belgrade, Serbia, 31. 10.–14. 11. 2012

Visiting researchers

- Dr. Ismael Fabregas, Centro de Investigaciones en Sólidos, CITEFA, Buenos Aires, Argentina, 1. 10.–31. 12. 2012
- Dr. Zoran Jovanović, Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, 10. 9.–31. 12. 2012
- 3. Dr. Lei Li, Zhejiang University, Hangzhou, China, 31. 8.-31. 12. 2012

STAFF

Researchers

- Asst. Prof. Boštjan Jančar
- Dr. Špela Kunej 2
- Dr. Marjeta Maček Kržmanc
- 4. Prof. Danilo Suvorov, Head
- Asst. Prof. Srečo Davor Škapin

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- Dr. Jakob König
- Dr. Uroš Kunaver* 9
- Dr. Manca Logar
- 10. Dr. Matjaž Spreitzer
- 11. Dr. Marko Udovič*
- 12. Dr. Asja Veber
- 13. Dr. Marija Vukomanović

Postgraduates

14. Dr. Ines Bračko, left 01.11.12

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ORIGINAL SCIENTIFIC ARTICLE

- 1. Mostafa Baghbanzadeh, Srečo D. Škapin, Zorica Crnjak Orel, C. Oliver Kappe, "A critical assessment of the specific role of microwave irradiation in the synthesis of ZnO micro- and nanostructured materials", Chemistry (Weinh., Print), vol. 18, issue 18, pp. 2724-2731, 2012
- 2. Anatolii Belous, Oleg V. Ovchar, Boštjan Jančar, Danilo Suvorov, "Microwave quality factor of cation-deficient perovskites $Ba(M_{1/3}^{2+}Nb_{2/3})O_3$ ", In: Proceedings of the MMA 2012, 7th International Conference on Microwave Materials and Applications, 3-6 June, 2012, Taiwan, Ferroelectrics, vol. 435, no. 1, pp. 166-175, 2012.
- 3. Mario Bianchetti, Ines Bračko, Srečo D. Škapin, Noemi E. Walsöe de Reca, "Nanocrystalline Tin oxide to be applied in a gas sensor", Sens. transducers, vol. 137, no. 2, pp. 155-164, 2012. 4. Mario Bianchetti, Marjeta Maček, Ines Bračko, Srečo D. Škapin, Noemi
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- 5. Mario Bianchetti, Marjeta Maček, Srečo D. Škapin, Noemi E. Walsöe de Reca, "Growth of well aligned tin oxide nanotubes by a sol-gel method", Sens. transducers, vol. 137, no. 2, pp. 189-198, 2012.
- 6. Igor Djerdj, Jasminka Popović, Jernej Stare, Gabriela Ambrožič, Srečo D. Škapin, Bojan Kozlevčar, Damir Pajić, Zvonko Jagličić, Zorica Crnjak Orel, "Nanocrystalline hybrid inorganic-organic one-dimensional chain systems tailored with 2- and 3-phenyl ring monocarboxylic acids", J. mater. chem., vol. 22, no. 20, pp. 10255-10265, 2012.
- 7. Igor Djerdj, Srečo D. Škapin, Miran Čeh, Zvonko Jagličić, Damir Pajić, Bojan Kozlevčar, Bojan Orel, Zorica Crnjak Orel, "Interplay between the structural and magnetic probes in the elucidation of thestructure of a novel 2D layered V₄O₄(OH)₂(O₂CC₆H₄CO₂)₄ DMF", *Dalton trans.* (2003. Print), vol. 41, issue 2, pp. 581-589, 2012.
- 8. Urban Došler, Marjeta Maček, Danilo Suvorov, "hase evolution and microwave dielectric properties of MgO - B2O3 - SiO2-based glassceramics", Ceram. int., vol. 38, issue 2, pp. 1019-1025, 2012.
- 9. Vilma Ducman, Vladimira Petrovič, Srečo D. Škapin, "Photo-catalytic efficiency of laboratory made and commercially available ceramic building products", Ceram. int., 2012.
- 10. Metka Hajzeri, Angela Šurca Vuk, Lidija Slemenik Perše, Marija Čolović, Bettina Herbig, Uwe Posset, Marjeta Maček, Boris Orel, "Sol-gel vanadium oxide thin films for a flexible electronically conductive polymeric substrate", In: Proceedings of the 9th International Meeting on Electrochromism, September 5-9, 2010, Bordeaux, France, Solar energy materials & solar cells, vol. 99, iss. 1, pp. 62-72, 2012.
- 11. Nataša Jović, Marija Prekajski, Aleksandar Kremenović, Boštjan Jančar, V. Kahlenberg, Bratislav Antić, "Influence of size/crystallinity effects on the cation ordering and magnetism of α -lithium ferrite

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15. Sonja Jovanović, B. Sc.

16. Dejan Klement, B. Sc.

17. Mario Kurtjak, B. Sc.

18. Mojca Otoničar, B. Sc.

19. Andreja Šestan, B. Sc.

22. Damjan Vengust, B. Sc.

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20. Tina Šetinc, B. Sc.

21. Vojka Žunič, B. Sc

Technical officers

- 12. Dragana Jugović, Miodrag Mitrić, Maja Kuzmanović, Nikola Cvjetićanin, Smilja Marković, Srečo D. Škapin, Dragan Uskoković, "Rapid crystallization of LiFePO4 particles by facile emulsion-mediated solvothermal synthesis", Powder technol., vol. 219, pp. 128-134, 2012.
- 13. Stanislav Kamba, Veronica Goian, Viktor Bovtun, Dmitri Nuzhnyy, Martin Kempa, Matjaž Spreitzer, Jakob Koenig, Danilo Suvorov, "Incipient ferroelectric properties of NaTaO₃", Ferroelectrics, vol. 426, no. 1, pp. 206-214, 2012.
- 14. Marta Kasunič, Srečo D. Škapin, Danilo Suvorov, Amalija Golobič, 'Polymorphism of LaTaTiO₆", *Acta chim. slov.*, vol. 59, no. 1, pp. 117-123 2012
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- 39. Marija Vukomanović, Vojka Žunič, Mojca Otoničar, Urška Repnik, Boris Turk, Srečo D. Škapin, Danilo Suvorov, "Hydroxyapatite/platinum biophotocatalyst: a biomaterial approach to self-cleaning", *J. mater. chem.*, vol. 22, no. 21, pp. 10571-10580, 2012.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

1. Sonja Jovanović, Matjaž Spreitzer, Mojca Otoničar, Danilo Suvorov, "Synthesis of cobalt ferrite nanoparticles using a combination of the co-precipitation and hydrothermal methods", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 234-240.

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- 4. Matejka Podlogar, Damjan Vengust, Nina Daneu, Jacob J. Richardson, Aleksander Rečnik, Slavko Bernik, "Influence of seed layer on the properties of ZNO films prepared by low-temperature hydrothermal synthesis", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 345-350.
- 5. Tina Šetinc, Matjaž Spreitzer, Špela Kunej, Danilo Suvorov, "Dielectric and ferroelectric properties of sol-gel-derived Na_{0.5}TiO₃ thin films", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 326-337.
- 6. Vojka Žunič, "Photocatalytic discoloration of the azo dye methylene blue in the presence ofirradiated TiO_2/Pt nano-composite", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 345-353.

PATENT APPLICATION

- 1. Aleš Dakskobler, Andraž Kocjan, Manca Logar, *Method for the preparation of carrier colloidal powder with high specific surface area*, W02012053990 (A2), World Intellectual Property Organization, 26.4.2012.
- 1. Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, *Functionalized* hydroxyapatite/gold composites as "green" materials with antibacterial activity and a process for preparing and use thereof, P-201200204, Urad RS za intelektualno lastnino, 15.6.2012.

PATENT

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- 2. Aleš Dakskobler, Andraž Kocjan, Manca Logar, *Method for the preparation of carrier colloidal powder with high specific surface area*, SI23580 (A), Urad RS za intelektualno lastnino, 26.6.2012.

MENTORING

- 1. Ines Bračko, *Synthesis and functionalisation of one-dimensional titanate-based nanostructures:* doctoral dissertation, Ljubljana, 2012 (mentor Danilo Suvorov; co-mentor Boštjan Jančar).
- Marija Vukomanović, Sonochemical synthesis and characterization of hydroxyapatite/metal-based composite materials for biomedical applications: doctoral dissertation, Ljubljana, 2012 (mentor Srečo Davor Škapin; co-mentor Dragan Uskoković).
- 3. Jože Katanec, *Antibacterial protections of refrigeration appliances:* master's thesis, Ljubljana, 2012 (mentor Danilo Suvorov; co-mentor Boštjan Pečnik).

DEPARTMENT OF BIOCHEMISTRY, MOLECULAR AND STRUCTURAL BIOLOGY B-1

The research activities of the members of the department are largely focused on studies of the physiological role of proteases in normal and pathological conditions, the mechanism of their action and regulation, as well as their properties and structure.

Protease research has undergone a major expansion in the past decade, largely due to the extremely rapid development of new technologies, such as quantitative proteomics and in-vivo imaging, as well as the extensive use of in-vivo models. These have led to the identification of physiological substrates and resulted in a paradigm shift from the concept of proteases as protein-degrading enzymes to proteases as key signalling molecules. Their catalytic activities are precisely regulated; the most important ways being zymogen activation and inhibition by their endogenous protein inhibitors. Any imbalance of this regulation can lead to pathologies such as autoimmune, neurological and cardiovascular disorders, cancer and osteoporosis. However, protease signalling pathways are only partially understood. We have only identified a minor subset of true physiological substrates for a limited number of proteases, and their physiological regulation is still not well understood. Similarly, links with other signalling Head: systems are not well established. The major challenges in protease research were therefore discussed in an invited **Prof. Boris Turk** review in EMBO Journal.



We have continued our work in the apoptosis field with a major focus on cysteine cathepsins. We have studied their potential role in the death receptor pathway, in order to clarify previous, contradictory findings. We have investigated apoptosis induced by tumour necrosis factor-related apoptosis-inducing ligand (TRAIL/Apo2L) and CD95 (Fas/APO-1) using four different cell lines, HeLa, HuH-7, Jurkat, and U-937. All four cell lines exhibited different levels of cathepsins and responded differently to apoptosis triggering. Jurkat cells were found to be the most sensitive

and the only ones that were sensitive to the agonistic anti-APO-1 antibody. Apoptosis was accompanied by caspase activation, loss of the mitochondria and lysosome integrity, and the release of cysteine cathepsins into the cytosol, as judged based on the hydrolysis of the cysteine cathepsin substrate Z-FR-AMC and by the immunological detection of cathepsin B. The inhibition of caspases by the broad-spectrum inhibitor Z-VAD-FMK prevented apoptosis, including the mitochondrial and lysosomal membrane permeabilization, as well as cathepsin release into the cytosol, consistent with caspases playing a crucial role in the process. Conversely, however, although the cathepsin selective inhibitors E-64d and Ca-074Me completely blocked the cathepsin activity, these inhibitors neither prevented apoptosis and its progression nor the mitochondrial and lysosomal membrane permeabilization associated with this type of cell death. Consequently, cathepsin release into the cytosol was also not prevented. Together, these data indicate that cysteine cathepsins are not required for the TRAIL- and CD95-mediated apoptosis in various human cancer-cell lines. However, it cannot be completely excluded that lysosomes and cysteine cathepsins are involved in the amplification, but not in the initiation, of death receptor-mediated apoptosis. In addition, we have shown that the overexpression of the endogenous cathepsin inhibitor stefin B in the nucleus of astrocytoma T98G cells delayed the activation of executioner caspases upon apoptosis induction with staurosporine. Since the cathepsin inhibitor E-64d did not prevent caspase activation, we concluded that the delay of caspase activation in T98G cells overexpressing



Figure 1: Tick inhibitor of human proteases in immune cells from host skin - Confocal microscopy with a white light laser (LEICA TCS SP5 X)

stefin B in the nucleus is independent of cathepsin inhibition. In collaboration with M. Goligorsky, we have found that cathepsins are involved in the stress-induced premature senescence (SIPS) of endothelial cells through the degradation of sirtuin-1. Finding that SIRT1 is an important substrate of cysteine cathepsins B, S, and L further suggests that this is a mechanism linking cell stress to apoptosis and SIPS. The proposed mechanism of SIRT1 depletion in stress has all of the attributes of being a paradigm of SIPS of endothelial progenitor cells. In addition, we contributed several review papers about the potential role of the lysosomal system and the cathepsins in apoptosis and apoptosis-related therapies.

More work has been carried out on understanding the protease function. Major histocompatibility class (MHC) II molecules are essential for running an adaptive immune response. They are produced in the ER and targeted to late endosomes with the help of invariant chain (Ii) trimers. Ii trimerization may be induced by the Ii TM domain. To enable mechanistic and structural studies of MHC class II-Ii assembly, soluble forms of the complexes were expressed. We show that Ii trimerizes in the absence of the transmembrane part, prior to the binding of α/β chains. The biochemical analysis supports the suggestion that the MHC class II-Ii complexes are not necessarily trimers of trimers, but that the Ii trimer can also be occupied by one or two MHC class II complexes.



Figure 2: Tick inhibitor of human proteases in immune cells from host skin - Confocal microscopy with white light laser (LEICA TCS SP5 X)

Also, the release of the thyroid hormone tyroxin from thyroglobulin is controlled by a complex regulatory system, involving several proteases. We have focused on dipeptidase cathepsin C and a metallopeptidase lysosomal dipeptidase (PGCP), which degrades dipeptides to amino acids. We have shown in *in vitro* experiments that cathepsin C removes up to 12 amino acids from the N-terminus of porcine thyroglobulin, including a dipeptide with thyroxin on position 5. The newly formed N-terminus, Arg-Pro-, was not hydrolysed further by cathepsin C. Secretion of the active cathepsin C and PGCP from FRTL-5 cells was found to be stimulated by TSH, insulin, and/or somatostatin. The released enzymes were found to liberate thyroxin from porcine thyroglobulin added to media. Furthermore, the hormone release could be reduced by synthetic inhibitors of cysteine and metalloproteinases, suggesting that cathepsin C and PGCP are involved in thyroglobulin regulation.

Another protease we have been working on was cathepsin E. A splice variant of cathepsin E was found to be expressed in a number of gastric carcinomas. Using polyclonal antibodies and biotinylated inhibitor pepstatin A, we have detected this cathepsin E variant in HeLa cells. When expressed, the splice variant was found to be inactive, in contrast to the full-length wild-type form, which was activated at acidic pH. A comparative structure model of the splice variant based on its alignment to the known structure of the cathepsin E intermediate enabled us to explain the loss of activity.

We have also continued our work on protease inhibitors. In collaboration with the group of Prof. Kos, we were involved in the characterization

of the serine protease inhibitor cospin from Coprinopsis cinerea. We have determined the crystal structure of the inhibitor, which revealed that the protein has a β -trefoil fold. Site-directed mutagenesis and mass-spectrometry results have confirmed Arg-27 as the reactive binding site for trypsin inhibition. The loop containing the Arg-27 residue is positioned between the $\beta 2$ and $\beta 3$ strands, distinguishing cospin from other β -trefoil-fold serine protease inhibitors in which $\beta 4$ - $\beta 5$ or $\beta 5$ - $\beta 6$ loops are involved in the protease inhibition. The overall results suggest that cospin and its homologs are effectors of a fungal defence mechanism against fungivorous insects that function by



Figure 3: IVIS Spectrum Pre-clinical In Vivo Imaging System is the first whole body imaging system in Slovenia.

the specific inhibition of serine proteases in the insect gut.

We participated in three FP7 projects, being the coordinators of one of them (LIVIMODE). We are also involved in two Slovenian Centers of Excellence, Center for Integrative approaches for Chemistry and Biology of Proteins (CIPKEBIP) that we also coordinate, and Nanosciences and Nanotechnologies. We are partners in the competence center BRIN, which, like both Centers of Excellence, brings together researchers from both industry and academia. In addition, there are numerous other international collaborations with excellent research teams from different countries including Belgium, France, Germany, Sweden, Switzerland, UK, USA, Australia and Japan, which resulted in joint publications. Prof. Vito Turk was invited to organize a special issue of Biochimica Biophysica Acta, dedicated to the Nobel laureate Christian de Duve and the 60 years since his discovery of the lysosome, which was a major honour. Several members of the department were invited to give lectures at international symposia and foreign universities.

Some important publications in the past year

- 1. Turk, B., Turk, D., Turk, V.: Protease signalling: the cutting edge. EMBO J. 31, 2012, pp. 1630-1643
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Organization of conferences and meetings

- 1. 29th Winter School on Proteinases and their Inhibitors, Recent Developments, Tiers, Italy, 29. 2.-4. 3. 2012, coorganizers
- 2. 13th International Symposium on Proteinases, Inhibitors And Biological Control, Portorož, 22.-26. 9. 2012

Patent granted

1. Matthew Bogyo, Steven H. L. Verhelst, Marko Fonović, Mild chemically cleavable linker system, US8314215 (B2), United States Patent and Trademark Office, 20.11.2012.

INTERNATIONAL PROJECTS

- 7. FP MICROENVIMET: Understanding and fighting metastasis by modulating the tumor microenvironment through interference with the protease network European Commission text Dec Older Vielling
- Asst. Prof. Olga Vasiljeva7. FP ALEXANDER: Mucus permeating nanoparticulate drug delivery systems European Commission
- Asst. Prof. Olga Vasiljeva 3. 7. FP - LIVIMODE: Light-based functional in vivo monitoring of diseases related enzymes European Commission Prof. Boris Turk
- MD simulations of the initial steps in oligomerization of an amyloidogenic protein human stefin B; in comparison to the less amyloidogenic stefin A Slovenian Research Agency
- Prof. Eva Žerovnik
- Nuclear inhibitors of cysteine proteinases influence heterochromatin distribution in the nucleus Slovenian Research Agency
- Slovenian Research Agency Asst. Prof. Nataša Kopitar - Jerala
- The role of cystatins in immune response to viruses Slovenian Research Agency Asst. Prof. Nataša Kopitar - Jerala

RESEARCH PROGRAMS

- Structural biology Prof. Dušan Turk
- Proteolysis and its regulation Prof. Boris Turk

R & D GRANTS AND CONTRACTS

1. Cell signalling of Toll-like receptors Asst. Prof. Nataša Kopitar - Jerala

VISITORS FROM ABROAD

- Georgy Mikhaylov, Siberian State Medical University, Tomsk, Siberia, Russia, 1. 1.-31. 12. 2012 (JSI Scholarship)
- 2. Dr. Michal Potempa, Jegiellonian University, Krakow, Poland, 23.-25. 1. 2012
- 3. Dr. Lawrence Banks, ICGEB, Trieste, Italy, 3. 2. 2012
- 4. Dr. Brigita Urbanc, Drexel University, Philadelphia, USA, 28. 2. 2012

- Secretory vesicle mobility and calcium homeostasis in astrocytes Prof. Veronika Stoka
- Study of hom(e)ologous recombination in the evolution of polyketide synthases Prof. Boris Turk
- 4. The role of small GTPases in the regulation of endosomal/lysosomal transport in astrocytes
- Prof. Veronika Stoka 5 Cathensin F: characterisation and biological role
- 5. Cathepsin E: characterisation and biological role Prof. Vito Turk
- The role of cysteine cathepsins and caspases in neurodegeneration Prof. Veronika Stoka
- 7. The role of lysosomea and lysosomal proteases in cellular signalling Prof. Boris Turk
- The role of cysteine cathepsins in cellular signalling Prof. Boris Turk
- Role and relevance of empirical geometric parameters in crystal structure determination of macromolecules for prediction of ligand binding Prof. Dušan Turk
- Involvement of the lysosomal cysteine peptidase inhibitors in progression and metastasis of mammary cancer Asst. Prof. Olga Vasiljeva
- Inhibitors of cysteine carboxypeptidases as regulators of autoimmune and neurodegenerative processes Asst. Prof. Olga Vasiljeva
- Oligomers of amyloidogenic proteins from a to z: biophysical properties, structure, function and mutual interactions Prof. Eva Žerovnik
- Research on new technologies for conservation restoration of baroque easel paintings Asst. Prof. Marko Fonović
- 14. XIII. International Symposium on Proteinases, Inhibitors and Biological Control Prof. Boris Turk
- 15. Competency centre for biotechnological development and innovation: CC BDI Prof. Boris Turk
- P2012, 13th International symposium on proteinases, inhibitors and biological control, Portorož, Slovenia, 22.–26. 9. 2012
 Prof. Boris Turk
- Prof. Kazuo Umezawa, Department of Molecular Target Medical Screening, School of Medicine, Aichi Medical University, Nagakute, Japan, 15.–16. 10. 2012
- Andrey Kadin, Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry Russian Academy of Science, Moscow, Russia, 15.–31. 12. 2012 (JSI Scholarship)

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- 13. Asst. Prof. Olga Vasiljeva
- 14. Asst. Prof. Tina Zavašnik Bergant
- 15. Prof. Eva Žerovnik

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- 16. Dr. Katarina Črnigoj Kristan, left 10.05.12
- 17. Dr. Saška Ivanova, left 01.09.12
- 18. Dr. Marko Mihelič
- 19. Dr. Petra Nikolić
- 20. Dr. Katarina Pegan
- 21. Dr. Cristina Gabriela Pinto Droga Mazovec
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- 23. Dr. Jure Pražnikar*
- 24. Dr. Miha Renko
- 25. Dr. Dejan Suban
- 26. Dr. Aleš Špes
- 27. Dr. Aleksandra Usenik
- Postgraduates
- 28. Katja Bidovec, B. Sc.

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- 2. Matjaž Brvar, Andrej Perdih, Miha Renko, Gregor Anderluh, Dušan Turk, Tomaž Šolmajer, "Structure-based discovery of substituted 4,5'bithiazoles as novel DNA gyrase inhibitors", *J. med. chem.*, vol. 55, issue 14, pp. 6413-6426, 2012.
- 3. Jun Chen, Sandhya Xavier, Eliza Moskowitz-Kassai, Robert Chen, Connie Y. Lu, Kyle Sanduski, Aleš Špes, Boris Turk, Michael S. Goligorsky, "Cathepsin cleavage of Sirtuin 1 in endothelial progenitor cells mediates stress-induced premature senescence", *Am J Pathol*, vol. 180, no. 3, pp. 973-983, 2012.
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Note: * part-time JSI member

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10. Vito Turk, Veronika Stoka, Olga Vasiljeva, Miha Renko, Tao Sun, Boris Turk, Dušan Turk, "Cysteine cathepsins: from structure, function and regulation to new frontiers", *Biochimica et biophysica acta, Proteins and proteomics*, vol. 1824, no. 1, pp. 68-88, 2012.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- 1. Nataša Mehle, Maja Ravnikar, Marina Dermastia, Petra Nikolić, Matevž Rupar, Tina Naglić, Gabrijel Seljak, Ivan Žežlina, Erika Orešek, "Novi podatki o razširjenosti zlate trsne rumenice v Sloveniji, biologiji prenašalca in obvladovanju bolezni", In: *Zbornik referatov*, 4. slovenski vinogradniško-vinarski kongres z mednarodno udeležbo, Nova Gorica, 25. & 26. 1. 2012 = 4th International Slovenian Congress on Vitiviniculture, Nova Gorica, Slovenia, 25. & 26. 1. 2012, Denis Rusjan, ed., Ljubljana, Biotehniška fakulteta, = Biotechnical Faculty, 2012, pp. 81-86.
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INDEPENDENT PROFESSIONAL COMPONENT PART OR A CHAPTER IN A MONOGRAPH

- 1. Mira Polajnar, Slavko Čeru, Nataša Kopitar-Jerala, Dejan Caglič, Eva Žerovnik, "Protein aggregation as a modulatory factor in EPM1", In: *Amyloids: composition, functions, and pathology*, Irene P. Halcheck, ed., Nancy R. Vernon, ed., Hauppauge, Nova Science Publishers, 2012, pp. 103-118.
- Tina Zavašnik-Bergant, "Quantification of immunogold labelling in two populations of dendritic cells: a study on endogenous protease inhibitor", In: *Current microscopy contributions to advances in science and technology*, (Microscopy book series, vol. 5), A. Méndez-Vilas, ed., Badajoz, Formatex Research Center, 2012, zv. 1, pp. 358-365.

PATENT

Matthew Bogyo, Steven H. L. Verhelst, Marko Fonović, *Mild chemically cleavable linker system*, US8314215 (B2), United States Patent and Trademark Office, 20.11.2012.

MENTORING

- 1. Dušana Majera, *Production and characterization of MHC class Il-invariant chain complex:* doctoral dissertation, Ljubljana, 2012 (mentor Dušan Turk; co-mentor Jacques Neefjes).
- 2. Dejan Suban, *Effect of N-glycosylation on plasma glutamate carboxypeptidase function:* doctoral dissertation, Ljubljana, 2012 (mentor Vito Turk; co-mentor Iztok Dolenc).
- 3. Aleš Špes, *Role and significance of cysteine cathepsins in TRAIL induced apoptosis:* doctoral dissertation, Ljubljana, 2012 (mentor Vito Turk; co-mentor Boris Turk).
- 4. Nina Vidergar, *Degradation of ataxin-3 and its mutants by cysteine cathepsins : a possible role of ataxin-3 fragments in spinocerebellar ataxia type 3:* master's thesis, Ljubljana, 2012 (mentor Veronika Stoka; co-mentor Boris Turk).
- 5. Irena Leonida Kropf, *Effect of lowering (percentage of) salt in meat products on the content of the number of microorganisms:* master's thesis, Maribor, 2012 (mentor Avrelija Cencič; co-mentor Livija Tušar).

DEPARTMENT OF MOLECULAR AND **R-2 BIOMEDICAL SCIENCES**

The research program of the Department of Molecular and Biomedical Sciences is focused on basic research in protein biochemistry, molecular and cellular biology, and genetics. The primary goal of our investigations is the acquisition of a new understanding of mammalian pathophysiology with the aim of improving human and animal health.

Secreted phospholipases A, (sPLA,s)

The major research topic of the department is the sPLA_s originating from animal toxins as well as those found in humans. We are studying the molecular mechanisms of the action of the toxic sPLA_s, particularly those endowed with presynaptic neurotoxicity, and the role of endogenous sPLA,s in the pathological and physiological processes in mammals.

By means of protein engineering and chemical synthesis we have prepared several new molecular tools for characterising sPLA, binding proteins, searching for novel receptors, studying the dynamics of the translocation of sPLA,s from the external space into the cells, the localization of sPLA,s inside cells and their co-localization with Head: already described binding proteins.

In 2012 we continued with intensive research on the molecular mechanism of the action of presynaptically neurotoxic sPLA,s. As model sPLA,s in our studies we used ammodytoxin (Atx) from the venom of the nose-horned

viper (Vipera ammodytes ammodytes), belonging to group IIA sPLA,s, and also OS₂ from the venom of the Australian taipan (Oxyuranus scutellatus scutellatus), which is a group I sPLA. We have been trying to answer several key questions about the action of this group of neurotoxic enzymes. We were

New substances and molecular tools to improve human and animal health.

interested in the identification of the N-type sPLA, receptor in the presynaptic membrane of a motoneuron, which is crucial for the expression of neurotoxicity. To trace this receptor we decided to use OS., which binds to it with a 1000-fold higher affinity than Atx. In the scope of an international bilateral project Proteus with a research group

from the Institute of Molecular and Cellular Pharmacology of the National Centre for Scientific Research (CNRS), Valbonne, France, we prepared large quantities of recombinant wild-type OS, from the venom of the Australian taipan and its chimera with a similar, but non-toxic, OS, from the venom of the same snake. In the following, their photo- reactive derivatives will be prepared, which are expected to enable the identification of the N-type receptor for sPLA_s in mammals.

Following demonstrations that sPLA₂s can also act inside cells, their intracellular activity became a very attractive research topic for numerous research groups. In our group these investigations have been conducted using different cellular models. In the past year we concluded an investigation of the molecular mechanism of the action of Atx in yeast Saccharomyces cerevisiae. Based on the results of an SGA (synthetic genetic array) analysis (Figure 1) and the analysis of the influence of cytosol-expressed Atx on the dynamics of sites of endocytosis in the plasma membrane (PM) of the yeast cell (Figure 2), we concluded that Atx significantly inhibits the process of endocytosis by inhibiting the function of amphiphysin. Amphiphysin is a protein that plays a key role in the final steps of the release of endocytotic vesicles from the PM. In the initial phase of Atx action on endocytosis, its binding to the 14-3-3 protein, located on the PM at the sites where endocytic vesicles start to form, is important. Afterwards, Atx phospholipase activity is crucial for the blocking effect (M. Mattiazzi et al., PLoS ONE, 7 (2012), e40931). In the future we will test the hypothesis, based on the results obtained in yeast, about the way of inhibiting the process of endocytosis by sPLA,s from the cytosol also in mammalian cells. Knowing how neurotoxic sPLA₂s act may open new approaches to the regulation of endocytosis, which would be extremely important for human medicine. The functional-genomic approach to genetic interactions between genes in a systematic manner.



Figure 1: Schematic representation of the synthetic genetic array (SGA) analysis method. SGA is a technique that enables the identification of the



Prof. Igor Križaj



Figure 2: The procedure to determine the lifetime and movement of an endocytic vesicle in a yeast cell. Kymograph (right) is obtained by dissecting through time a particular area of the yeast plasma membrane (blue circle) using real-time fluorescence microscopy.

study the molecular mechanisms of action of animal toxins in the yeast cell, introduced by our group in the field of toxinology, obviously attracted considerable attention – the editor of Toxicon, the main toxinology journal, invited us to prepare a review paper on this topic (M. Mattiazzi et al., *Toxicon*, 60 (2012) 558–571). Intensive research on the intracellular action of Atx also proceeded with two mammalian cell lines, mouse NSC34 and rat PC12 cells. Using confocal microscopy we observed the dynamics of the internalization of Atx into the PC12 cells. Among other experiments in these

cells, we also confirmed the co-localization of Atx with mitochondria (Figure 3). It is presumed that the interaction of certain sPLA₂s, including Atx, with calmodulin (CaM), a regulatory protein in the cytosol, is physiologically very important. Therefore, we study this interaction with particular interest. Aiming to observe the dynamics of the interaction between Atx and CaM in the cell using a FRET method, we were developing fluorescence derivatives of both proteins in the past year. We were also very interested in a detailed structural analysis of the interaction between Atx (and homologous mammalian sPLA₂s) and CaM, as well as in the interaction of the sPLA₂–CaM complex with the phospholipid membrane, which will be accomplished by using protein NMR spectroscopy. To this end we prepared in the scope of a postdoctoral research project the recombinant ¹³C- in ¹⁵N-labelled Atx and CaM. In 2012 we acquired the first NMR spectra. In the NMR studies we collaborate with two partner groups, the Bijvoet Centre from the Utrecht University, Netherlands, and the NMR centre from the National Institute of Chemistry, Ljubljana, Slovenia. With the results obtained already we succeeded to raise additional funds from the European project FP7-Bio-NMR to cover the expenses of the NMR measurements at Utrecht University.

We concluded a bilateral project with Bulgarian colleagues from Sofia University. In the scope of this project we looked for the differences in the mechanism of neurotoxic action of monomeric Atx from the venom of our subspecies of the nose-horned viper (*Vipera a. ammodytes*) and the two-chain vipoxin from the snake venom of the Bulgarian subspecies (*Vipera a. meridionalis*). The data obtained, leading to the conclusion that, in spite of



Figure 3: Co-localization of Atx and mitochondria in PC12 cells. Cells were incubated with fluorescently labelled AtxA (red signal) and a marker specific for mitochondria (green signal). Using a confocal microscope at 100-fold magnification we acquired 13 optical slices. In silico, these were then assembled into a tri-dimensional image. The yellow signal corresponds to areas where AtxA and mitochondria are co-localized.

the high structural identity between Atx and vipoxin, the mechanisms of their neurotoxic action differ substantially, are being prepared for publication.

There is a common problem in many of the early studies of isolated snake venom sPLA,s - the results obtained may not be reliable, particularly when there is a reasonable doubt as to whether the toxins tested were completely pure. AtxA is the most toxic sPLA, of three isotoxins with presynaptic neurotoxicity of the nose-horned viper, with an LD₅₀ of 21 mg/kg in mice. The toxicity of AtxA, purified from the viper's venom, has been confirmed by that of recombinant AtxA, prepared by protein engineering in a bacterial expression system of Escherichia coli. We have also re-evaluated the toxic potencies of two other isoforms, AtxB and AtxC, by using highly purified recombinant proteins. It has been shown that their intraperitoneal LD_{co}s, determined as 960 mg/kg for AtxB and 310 mg/kg for AtxC, differ significantly from the values previously reported for these isoforms isolated from the snake venom (P. Prijatelj-Žnidaršič and J. Pungerčar, Toxicon, 6 (2012), 642-643). Our results also point to an even more important role of the Tyr115/Ile116/ Arg118/Asn119 cluster in the neurotoxicity of Atxs and similar toxins than previously thought. At the end of last year we also completed and submitted for publication a study of the putative involvement of free arachidonic acid, released as a result of the enzymatic activity of AtxA, in apoptotic changes of montoneuron-like cells.

Several sPLA₂ enzymes have been implicated in the pathology of cancer, with roles in either tumour promotion or inhibition, depending on irrepresent of the tumour involved. The group X sPLA (sPLA X) efficiently

the tissue and biochemical microenvironment of the tumour involved. The group X sPLA₂ (sPLA₂-X) efficiently released fatty acids and lysophospholipids from various cells and stimulates colon-cancer cell proliferation in an enzymatic activity-dependent manner. In order to elucidate a possible role of sPLA₂-X in breast cancer, we analysed the effects of exogenously-added recombinant sPLA₂-X on the viability, proliferation and survival of model breast-cancer cell lines with different tumourigenicity. Already low nanomolar concentrations of exogenously added

recombinant sPLA,-X stimulated the proliferation of highly invasive breast-cancer cells, but decreased the viability of weakly and moderately tumorigenic cells. The positive effect on breast-cancer cell proliferation was confirmed with ectopically expressed sPLA₂-X as well. Importantly, the proliferative effect was strictly dependent on the PLA₂ enzymatic activity, as it was completely abolished by the pan-sPLA, inhibitor varespladib. Furthermore, the critical role of the enzymatic activity was confirmed in experiments with the exogenously-added, enzymatically inactive, active-site mutant of sPLA,-X as well as with the forcible expression of the same mutant in breast-cancer cells. Since the positive effect on cell proliferation was more significant in starved cells, we asked if sPLA,-X also exerts an anti-apoptotic role in severely starved cells. Indeed, exogenously added as well as ectopically expressed sPLA,-X prevented serum-withdrawal-induced cell death of the highly invasive breast-cancer cells. The effect was strictly

dependent on sPLA, enzymatic activity and was most significant in the highly invasive MDA-MB-231 and T-47D breast cancer cells and absent in the weakly tumourigenic MCF-7 cells (Figure 4). It has been shown previously that exogenously added oleic acid prevents serum-withdrawal-induced apoptosis most significantly in MDA-MB-231 and T-47D cells. The pro-survival action of the oleic acid was linked to the particular ability of these two cell lines to accumulate large amounts of triglycerides in lipid droplets. Since oleic acid is one of the major products of sPLA₂-X cell membrane hydrolysis, we reasoned that sPLA₂-X might affect the lipid cycling and accumulation as well as prolonging the survival of breast-cancer cells. Indeed, we found Figure 4: Human sPLA2-X conveys a significant survival advantage that sPLA₂-X induced lipid droplet formation in the serum-starved as well as in proliferating cells in an enzymatic activity-dependent manner. Using a range of cell signalling and lipid metabolism inhibitors we found that fatty acid activation, mitochondrial fatty acid oxidation and AMP-activated varespladib completely abolished its effect on cell survival. protein kinase, a key regulator of cellular lipid metabolism, are involved in



only to the highly invasive breast-cancer cell line MDA-MB-231. Cells of five breast-cancer cell lines were serum-starved and treated in a serumfree medium with sPLA2-X for 96 h before a flow cytometric analysis of the apoptosis. The inhibition of enzymatic activity sPLA2-X with

both the pro-survival and lipid droplet-inducing effects of sPLA,-X. The pro-survival and anti-apoptotic signalling is associated with changes in the lipid storage and fatty acid metabolism. The effects of sPLA,-X on the growth and survival of breast-cancer cells reveal previously unknown connections between the sPLA₂-mediated fatty acid release and alterations of lipid metabolism in cancer.

Another aspect of our research on the involvement of human sPLA, s in disease is the mechanisms of regulation for sPLA, gene expression. Since tumours depend on aberrant epigenetic modifications that enable their growth and survival, we wanted to determine the involvement of DNA methylation and histone acetylation in the regulation of sPLA, expression in a panel of cell line models of breast cancer. The treatment of cells with a DNA-methyltransferase inhibitor led to a significant increase in the expression of group IIA, III and X sPLA, s, indicating that DNA hypermethylation is responsible for sPLA, silencing in breast-cancer cells. Bisulphite sequencing of sPLA, promoter regions and the treatment of cells with transcription factor inhibitors suggested that Sp1, estrogen receptor alpha (ER-a), retinoic acid receptor alpha (RAR-a) and sterol segulatory element-binding protein (SREBP) transcription factors are crucial for sPLA, silencing by hypermethylation. Furthermore, the expression of group IIA, III and X sPLA_s was restored in cells treated with a histone deacetylase inhibitor, particularly in the most tumourigenic cell line used, and it was even further augmented upon inhibiting both cellular DNA methyltransferases and histone deacetylases. Our results clearly show that both DNA hypermethylation and histone acetylation are involved in the sPLA, gene silencing in breast-cancer cells, particularly in highly tumourigenic and invasive cells, and suggest the functional importance of these enzymes in malignant cell transformation.

Other pharmacologically active components from natural toxins

In the past year we continued the intensive study of the components of the nose-horned viper venom that affect the coagulation of blood - haemostasis. In the scope of a national research project we systematically evaluated, with our partners from the University Medical Centre Ljubljana, Division of Pediatrics, the influence of isolated venom components on different parts of the human haemostatic system. In this process we selected several venom proteins for further in-depth analysis. We concluded with the experimental work on the description of one of the major haemorrhagic molecules in the venom, homodimeric metalloproteinase (SVMP) VaH3 (Figure 5), and practically finished the analysis of another haemorrhagic SVMP, VaH4, which is a heterodimeric protein. The results are now being prepared for publication. Due to conspicuous achievements in the research on haemostasis and haemostasis-related pathologies we were invited to give an interview that was published in a prominent American journal Circulation (I. Križaj, Circulation, 126 (2012), f5-f6).

For many years we have been collaborating successfully with our colleagues from the Institute of Immunology in Zagreb, Croatia, on the development of procedures for the production of more effective antivenoms and methods for the testing of their quality. In 2012 we jointly published a study which reported that using the standard antivenom



Figure 5: Tri-dimensional model of VaH3, the haemorrhagic snake venom metalloproteinase from the venom of the nose-horned viper. The model represents a valuable instrument to study the structure-function relations of ADAM/ADAMTS, a homologous family of mammalian proteins with high therapeutic potential.

quality test on mice one cannot establish the content of the antibodies in the antiserum that are able to neutralize haemorrhagins in the nose-horned viper's venom. In other words, the standard mouse test is inadequate for human medicine (T. Kurtović et al., *Toxicon* 59 (2012), 709–717).

As one of the 20 partners in the EU 6FP integrated project "Conco" we have been involved in the analysis of the genome, transcriptome and venom proteome of the piscivorous marine snail *Conus consors* and related snails. In 2012, when this project was concluded, we succeeded in publishing two papers on the proteomic analysis of the high-molecular-mass (HMM) protein components isolated from the so-called "dissected" and "injected" venoms of *C. consors* (Figure 6). In this analysis we discovered proteins that define new protein families of an unknown biological function. It is particularly interesting that some of these new conoproteins are highly represented and appear to be present exclusively in cone snails (genus *Conus*). Derived complete or at least partial sequences of these structurally unique proteins will enable a study of their biological roles. The analysis of venom duct and salivary gland

EST libraries has also demonstrated differential expression sites of *C. consors* venom HMM proteins. Collectively, our results enabled a better understanding of the biological role of the HMM in the venom of cone snails (A. Leonardi et al., *Journal of Proteome Research*, 11 (2012), 5046–5058; A. Violette et al., *Marine Drugs* 10 (2012), 258–280).

High-throughput genetics and functional genomics in yeast Saccharomyces cerevisiae

Obesity and the resulting type-2 diabetes are a pressing health-related problem of today's societies, both in developed and developing countries. The biology of the changes in metabolism leading to obesity and diabetes is, however, not well understood. Insulin is the most important hormone to regulate sugar metabolism, but other hormones, such as adiponectin, play additional roles and also affect the metabolism-related disorders like diabetes. Specifically, adiponectin suppresses type-2 diabetes.

Zinc is an essential mineral that has also been implicated in the development of diabetes. It is required for the formation of insulin hexamer, the storage form of the hormone, and is thus important for the synthesis, storage, proper conformation and excretion of insulin from the pancreatic β -cells. Zinc depletion in humans can therefore lead to insulin production and secretion disorders, and hyperglycemia results in increased secretion and decreases in total the body zinc. The connection between diabetes and zinc is complex and still without a clear cause-and-effect relationship. Using yeast as a model system we have analyzed the genetic interactions of zinc depletion and overload, and in this context we additionally analyzed the role of the homologues of adiponectin receptor, yeast Izh proteins. It has been shown that the effects of Izh deficiency and zinc depletion overlap, and that both exert a



Figure 6: Workflow of Conus consors snail venom proteomics analysis. The study opened a way to understanding the biological roles of the high-molecular-mass proteins in the venom. We also discovered new families of proteins and the deduced amino acid sequences will enable clarification of their functions. The figure is reproduced from A. Leonardi et al., Journal of Proteome Research, 11 (2012), 5046–5058.

response typical of membrane fluidity changes. Using novel bioinformatics tools, we identified a modular nature of cellular responses to environmental or genetic perturbations. We thus demonstrated that Zn^{2*} concentration modulation is potentially useful in preventing and possibly also treating diabetes. However, rather than having a direct, diabetes-related target, it elicits an effect that resembles the inverse of the effects that occur as a consequence of a non-healthy lifestyle leading to diabetes.

Red-spotted newt (*Notophthalmus viridescens*) specimens from various locations in Canada and the USA were analyzed for the presence of tetrodotoxin (TTX) and its analogues (M. Yotsu-Yamashita et al., *Toxicon*, 59 (2011), 257–264). Considerable individual variations in toxin levels were found within and among the populations. TTX and its analogues were absent in efts and adults from the northernmost locations of the newt, and in adults from Florida. Newts kept in captivity for several years and reared on a toxin-free diet lost their toxicity. Bayesian and maximum likelihood phylogenetic analysis of specimens from the various populations using three phylogenetic markers (COI, ND2 and 16S RNA) revealed that populations from the northern states of the USA and Canada are genetically homogenous, whereas

the newts from Florida exhibited a much higher level of genetic divergence. This analysis has demonstrated that TTX-bearing populations are not genetically separated from those that lack TTX. Therefore, an exogenous source of TTX in the newts either *via* the food chain or its synthesis by symbiotic bacteria was suggested to explain the high variability and the lack of TTX in certain populations.

In an invited review we summarized the current understanding of intron gain in mammals (D. Kordiš and J. Kokošar, International Journal of Evolutionary Biology, 2012 (2012), e278981). Domesticated genes, originating from retroelements or from DNA-transposons, constitute an ideal system for testing the hypothesis on the absence of intron gain in mammals. Since single-copy domesticated genes originate from the intronless multicopy transposable elements, the ancestral intron state for domesticated genes is zero. A phylogenomic approach has been used to analyse all the domesticated genes in mammals and chordates that originated from the coding parts of transposable elements. A significant amount of intron gain was found only in domesticated genes of placental mammals, where more than 70 cases were identified (Figure 7). De novo gained introns show a clear positional bias, since they are distributed mainly in 5' UTR and coding regions, while 3' UTR introns are very rare. In the coding regions of some domesticated genes up to 8 de novo gained introns have been found. Surprisingly, the majority of intron gains have occurred in the ancestor of placental mammals. Domesticated genes thus represent an excellent system to study the mechanisms that allow the entry of newly formed introns in genes of placental mammals.

In an invited review we summarized the current understanding of the repetitive landscape of sauropsid genomes (D. Kordiš, *Evolutionary Biology: Mechanisms and Trends*, (2012); Heidelberg, New York, Dordrecht, London. Springer, pp. 243–263). Investigations of transposable elements (TEs) in sauropsid genomes over the past four decades have provided an insight into



Figure 7: Numbers of transposable element-derived gene domestication events and intron gains mapped on the chordate phylogenetic tree. In the superorder Boreoeutheria some additional intron gains have occurred. The figure is reproduced from D. Kordiš and J. Kokošar (2012), International Journal of Evolutionary Biology, 2012 (2012), 278981-1-278981-7.

the TE repertoires of all major extant sauropsid lineages. Invaluable information concerning the diversity, activity, and repetitive landscapes in sauropsids has emerged from the analyses of the chicken and *Anolis* (lizzard) genomes and other preliminary reptilian genome sequencing projects. Avian and reptilian genomes differ significantly in the classes of TEs present, their fractional representation in the genome and with the level of TE activity. While lepidosaurian genomes contain many active TE families, the extant avian genomes have few active TE lineages. Most reptilian genomes possess quite rich TE repertoires that differ considerably from those of birds and mammals. In sauropsid genomes, TEs have been active for more than 300 million years, and as such have had a large impact on the genetic diversity and genome architectures.

Other subjects

In 2012 we also worked on several projects out of the thematic scope of our department. We collaborated intensively with colleagues from the Department of Biology, Biotechnical Faculty, University of Ljubljana. With a structural analysis we participated in the determination of the mode of action of membrane-active proteins from the mushroom *Pleurotus ostreatus*. The conclusion of this study was that pleurotolysin B obligatory requires the presence of another protein ostreolysin A to form a pore in the membranes rich in cholesterol and sphingomyelin. The publications are in preparation. Together with the same group we also prepared a review paper about the use of pore-forming toxins during the sensing and labelling of membrane microdomains (M. Skočaj et al., Current Medicinal Chemistry, in press). A very important joint project in 2012 was dedicated to developing an original approach against bacterial infections. In the evolvement of the resistance of bacteria against antibiotics their SOS system is of crucial importance. The key role in the bacterial SOS response is played by a complex formed between a single-stranded DNA (ssDNA) and two bacterial proteins, RecA and LexA. Based on experimental data we build a tri-dimensional model of the complex ssDNA-RecA-LexA that will enable a design of substances to prevent development of bacterial resistance to antibiotics. The publication is in preparation.

In collaboration with the NMR Centre from the Utrecht University we prepared a chapter in a scientific monograph (L. Kovačič in R. Boelens, NMR of Biomolecules: Towards Mechanistic Systems Biology, (2012); Weinheim, Chichester. Wiley-VCH, pp. 239–252). In addition, by performing surface plasmon resonance (SPR) measurements, we studied together with this group, the mechanism of binding of structure-specific endonuclease ERCC1/XPF on DNA in the process of its repair.

Some outstanding publications in the past year

 Mattiazzi, M., Sun, Y., Wolinski, H., Bavdek, A., Petan, T., Anderluh, G., Kohlwein, S.D., Drubin, D., Križaj, I. and Petrovič, U.: A neurotoxic phospholipase A2 impairs yeast amphiphysin activity and reduces endocytosis. PLoS ONE 7, 2012, e40931

- 2. Jenko-Pražnikar, Z., Petan, T. and Pungerčar, J.: Ammodytoxins efficiently release arachidonic acid and induce apoptosis in a motoneuronal cell line in an enzymatic activity-dependent manner. NeuroToxicology, 2012, in press
- Leonardi, A., Biass, D., Kordiš, D., Stöcklin, R., Favreau, P. and Križaj, I.: Conus consors snail venom proteomics unveils functions, pathways and novel families involved in its venomic system. J. Proteome Res. 11, 2012, pp. 5046–5058
- Violette, A., Leonardi, A., Piquemal, D., Terrat, Y., Biass, D., Dutertre, S., Noguier, F., Ducancel, F., Stöcklin, R., Križaj, I. and Favreau, P.: Recruitment of glycosyl hydrolase proteins in a cone snail venomous arsenal: further insights into biomolecular features of Conus venoms. Mar. Drugs 10, 2012, pp. 258–280
- Mattiazzi, M., Petrovič, U. and Križaj, I.: Yeast as a model eukaryote in toxinology: a functional genomics approach to the studies of the molecular basis of action of pharmacologically active molecules. Toxicon 60, 2012, pp. 558–571

1.

2.

INTERNATIONAL PROJECTS

- 6. FP CONCO: Applied venomics of the Cone Snail species *Conus consors* for the accelerated, cheaper, safer and more ethical production of innovative biomedical drugs European Commission Prof. Igor Križaj
- Structural explanation of the high increase in enzymatic activity of secreted phospholipases A2 in complex with calmodulin by high resolution NMR Utrech University, Faculty of Science Dr. Lidija Kovačič
- Changes in spatiotemporal dynamics of endocytosis upon membrane pertubation Slovenian Research Agency Prof. Igor Križaj
- A genome-scale approach to maximization of triacylglycerol biosynthesis in yeast Slovenian Research Agency Prof. Igor Križaj
- Comparative study of two structurally diverse neurotoxic phospholipases A2, ammodytoxin from the Long-Nosed Viper (*Vipera ammodytes ammodytes*) and vipoxin from the Bulgarian Sand Viper (*Vipera ammodytes meridionalis*) venoms Slovenian Research Agency Prof. Icor Križai
- Towards the identification of N-type sPLA2 receptors Slovenian Research Agency Prof. Jože Pungerčar

RESEARCH PROGRAM

1. Toxins amd biomembranes Prof. Igor Križaj

VISITORS FROM ABROAD

- Sílvia Henriques, Instituto Superior Técnico, Lisbon, Portugal, 16. 3.–20. 4. 2012
 Prof. Michael Hanscho, Asst. Prof. Klaus Natter, University of Graz, Austria, 19.–20. 4. 2012
- 3. Asst. Prof. Klaus Natter, University of Graz, Austria, 16.-17. 7. 2012
- 4. Asst. Prof. Klaus Natter, University of Graz, Austria, 10.-11. 12. 2012

Antiretroviral APOBEC3 proteins and their role in retroelement defense Prof. Igor Križaj Photostability of selected industrial chemicals and their influence on the environment Asst. Prof. Uroš Petrovič

R & D GRANTS AND CONTRACTS

- Data and knowledge integration methods for network systems biology Asst. Prof. Uroš Petrovič
- Apoptotic effects of alkylpyridinium compounds on lung adenocarcinoma cells Prof. Igor Križaj
- Molecular description of lipid membrane changes in disease Prof. Igor Križaj
- Regulatory genomics: origin and evolution of the complex transcriptional regulatory network in vertebrates Asst. Prof. Dušan Kordiš
- Discovering innovative drugs for regulation of haemostasis by venomics of the Vipera ammodytes ammodytes snake Prof. Igor Križaj
- Pathogenomics and systems biology of new virulence factors in pathogenic bacteria Asst. Prof. Dušan Kordiš
- Structural explanation of the high increase in enzymatic activity of secreted phospholipases A2 in complex with calmodulin by high resolution NMR Dr. Lidija Kovačič

- 5. Dr. Tihana Kurtović, Institute of Immunology, Zagreb, Croatia, 24.–29. 9. 2012
- Dr. Gerard Lambeau, Institute de Pharmacologie Moleculare et Cellulare, Universite Nice, Sophia Antipolis, France, 19.–23. 10. 2012
- 7. Prof. Rolf Boelens , University of Utrecht, Utrecht, The Netherlands, 16. 11. 2012

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- 11. Minca Ferlin, B. Sc.
- 12. Petra Kaferle, B. Sc., left 01.08.12
- 13. Janez Kokošar, B. Sc.
- 14. Jernej Oberčkal, B. Sc.
- 15. Anja Pucer, B. Sc.
- 16. Tamara Sajevic, B. Sc.

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ORIGINAL SCIENTIFIC ARTICLE

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- Adrijana Leonardi, Daniel Biass, Dušan Kordiš, Reto Stöcklin, Philippe Favreau, Igor Križaj, "Conus consors snail venom proteomics proposes functions, pathways and novel families involved in its venomic system", *Journal of proteome research*, vol. 11, no. 10, pp. 4765-5108, 2012.
- Mojca Mattiazzi, Yidi Sun, Heimo Wolinski, Andrej Bavdek, Toni Petan, Gregor Anderluh, Sepp D. Kohlwein, David Drubin, Igor Križaj, Uroš Petrovič, "A neurotoxic phospholipase A₂ impairs yeast amphiphysin activity and reduces endocytosis", *PloS one*, vol. 7, iss. 7, pp. 1-13, e40931, 2012.
- 4. Petra Prijatelj, Jože Pungerčar, "A recent evaluation of the lethal potencies of ammodytoxins", *Toxicon (Oxford)*, vol. 59, no. 6, pp. 642-643, 2012.
- Katherine E. Tansey *et al.* (30 authors), "Genetic predictors of response to serotonergic and noradrenergic antidepressants in major depressive disorder : a genome-wide analysis of individual-level data and a meta-analysis", *PLoS medicine*, vol. 9, no. 10, str. e1001326-1e1001326-10, 2012.
- 6. Aude Violette, Adrijana Leonardi, David Piquemal, Yves Terrat, Daniel Biass, Sebastien Dutertre, Florian Noguier, Frederic Ducancel, Reto Stöcklin, Igor Križaj, Philippe Favreau, "Recruitment of glycosyl hydrolase proteins in a cone snail venomous arsenal: further insights into biomolecular features of conus venoms", *Mar. drugs*, vol. 10, no. 2, pp. 258-280, 2012.
- Mari Yotsu-Yamashita, John Gilhen, Ronald W. Russell, Kenneth L. Krysko, Christian Melaun, Alexander Kurz, Silke Kauferstein, Dušan Kordiš, Dietrich Mebs, "Variability of tetrodotoxin and of its analogues in the red-spotted newt, Notophthalmus viridescens (Amphibia: Urodela: Salamandridae)", *Toxicon (Oxford)*, vol. 59, no. 2, pp. 257-264, 2012.

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19. Darja Žunič Kotar

REVIEW ARTICLE

- 1. Dušan Kordiš, Janez Kokošar, "What can domesticated genes tell us about the intron gain in mammals?", *International Journal of Evolutionary Biology (Print)*, vol. 2012, pp. 278981-1-278981-7, 2012.
- 2. Mojca Mattiazzi, Uroš Petrovič, Igor Križaj, "Yeast as a model eukaryote in toxinology: a functional genomics approach to studying the molecular basis of action of pharmacologically active molecules", *Toxicon (Oxford)*, vol. 60, no. 4, pp. 558-571, 2012.

INDEPENDENT SCIENTIFIC COMPONENT PART OR A CHAPTER IN A MONOGRAPH

- 1. Dušan Kordiš, "The repetitive landscape of sauropsid genomes", In: *Evolutionary biology: mechanisms and trends*, Pierre Pontarotti, ed., Berlin [etc.], Springer Berlin, 2012, pp. 243-263.
- Lidija Kovačič, Rolf Boelens, "Protein DNA interactions", In: NMR of biomolecules: towards mechanistic systems biology, Ivano Bertini, ed., Kathleen S. McGreevy, ed., Giacomo Parigi, ed., Weinheim, Chichester, Wiley-VCH, 2012, pp. 239-252.

ENCYCLOPAEDIA, DICTIONARY, LEXICON, MANUAL,

ATLAS, MAP

1. Veronika Abram, Bronislava Črešnar, Marko Dolinar, Peter Dovč, Radovan Komel, Irina Milisav, Tomaž Sajovic, Igor Štern, Tom Turk, Marija Žakelj-Mavrič, Franc Gubenšek, Blagajana Herzog-Velikonja, Roman Jerala, Igor Kregar, Jože Pungerčar, Maksimiljan Sterle, Angleško-slovenski slovar izbranih izrazov iz biokemije in molekularne biologije, Ljubljana, Slovensko biokemijsko društvo, 2012.

MENTORING

1. Borut Jerman, *Role and action of endogenous secreted phospholipases* A_2 *in a motor neuron cell line:* doctoral dissertation, Ljubljana, 2012 (mentor Jože Pungerčar).
DEPARTMENT OF BIOTECHNOLOGY R-3

At the Department of Biotechnology we investigate biological molecules of microbiological, fungal, plant and animal origin using modern biotechnological methods. We would like to apply them for diagnostic and therapeutic purposes in human and veterinary medicine, for plant protection, the preparation of high-quality and safe food and for the protection of the environment, contributing to an improvement in peoples' health and of the environment in which we live. Our research work is focused on the processes of cancer progression and immune response, neurodegenerative processes, the biology of fungi, plant stress response and the search for new biotechnological approaches and products.

In 2012 the research on protease inhibitors from mushrooms was continued in view of their applicability. Cysteine protease inhibitors, mycocypins, and the trypsin inhibitor, cnispin, which we have thoroughly characterized in previous years, were used as ligands in affinity chromatography for the isolation of proteases from different complex sources. After the optimisation of the preparation and isolation procedures using Sepharose as support Head: we developed a similar method using monoliths as solid support in collaboration with BIA Separations d.o.o. and Prof. Janko Kos described both in the chapter of a book "The value of fungal protease inhibitors in Affinity Chromatography". Furthermore, inhibitors of cysteine proteases, macrocypins, were evaluated as potential pesticidal agents against herbivorous insects. In collaboration with the National Institute of Biology we used the potato and Colorado potato beetle as a model to show that macrocypins have a negative effect on the growth and development of Colorado

potato beetle larvae. Since this was the first demonstration of the potential application of proteins from mushrooms in plant protection against Colorado potato beetle we submitted an international patent application "Use of macrocypins as pesticidal agents" (PCT/EP2012/065373). In addition, besides other publications, we have published a review article covering the riches, unique characteristics and applicability of proteins from mushrooms in the renowned journal Trends in Biotechnology.

Macrocypins have a negative effect on the growth and development of the Colorado potato beetle larvae – international patent application PCT/ EP2012/065373.

In the field of glycobiology, we continued studying lectins, a diverse group of carbohydrate-binding proteins, and their biological activity from different mushroom species, i.e., clouded agaric (Clitocybe nebularis), parasol mushroom (Macrolepiota procera) and St. George's mushroom (Calocybe gambosa). In various cell lines we have been searching for the target glycoproteins of CNL, a lectin from C. nebularis, which have shown immunomodula-

tory and insecticidal properties. For this lectin we have shown the targets in human leukaemic T lymphocytes (Jurkat cell line), on which the lectin exerted an antiproliferative effect. Using confocal microscopy, we found CNL predominantly bound to the cell membrane of the Jurkat cells.

Several recombinant isolectins of sucrose-binding lectin from C. nebularis, CnSucL, were also prepared, which showed bactericidal and insecticidal actions. The latter effect corresponds to the binding specificity of the lectin for carbohydrates containing the Man3GlcNAc2 motif found in insects. A similar binding specificity was also shown for a lectin isolated by asialofetuin-Sepharose from C. gambosa, named gambosin, suggesting its defence function in the mushroom against insects.

Moreover, a recombinant lectin from *M. procera*, MpL, was expressed in E. coli, which showed a similar carbohydrate-binding specificity on glycan microarray analysis compared to

the lectin isolated from mushroom, i.e., for N'-acetyllactosamine (LacdiNAc) or di-LacNAc. In collaboration with ETH Zürich, the high toxicity of MpL was shown against *Caenorhabditis elegans* nematode, which contains

glycans specific for the lectin. A three-dimensional structure of this ricin-like lectin in a complex with its specific glycans was also obtained. MpL adopts a β-trefoil fold based on which the noncarbohydrate-binding mutants were constructed and prepared. We have also demonstrated the influence of MpL on the adhesion of U-937 monocytes and shown by confocal microscopy that MpL predominantly binds to the cell membrane and partially internalizes

Figure 1. Transgenic mice overexpressing wild-type human FUS develop an aggressive phenotype of amyotrophic lateral sclerosis.

Bivalent carbohydrate binding is required for the biological activity of CNL, the LacdiNAc (GalNAc[beta]1-4GlcNAc)-specific lectin from basidiomycete Clitocybe nebularis.



the cell. Using affinity chromatography on various sugars, several fungal lectins have been isolated – a ricin B-like lectin (CNL), sucrose-specific (CnSucL) and Sepharose-specific lectin (CnSepL) from the mushroom clouded agaric

Cospin and its homologs are effectors of a fungal defence mechanism against fungivorous insects.

(*Clitocybe nebularis*) and a LacNAc-specific ricin B-like lectin (MpL) and a galectin from the parasol mushroom (*Macrolepiota procera*). The lectins were characterized biochemically and the nucleotide sequences of their genes and cDNAs were determined to produce recombinant proteins expressed in the bacteria Escherichia coli.

The investigation of the role of proteases and protease inhibitors in malignant, immune and neurodegenerative processes was focused on natural killer (NK) cells in 2012. In collaboration with the group of prof. Jewett from UCLA we studied the role of cysteine proteases in the regulation of cytotoxicity in NK cells. We showed that freshly

isolated primary NK cells induce apoptosis in differentiated carcinoma cells and cancer stem cells, while anti-CD16 antibody and monocytes induce functional split anergy of NK cells by decreasing the cytotoxic function of NK cells and increasing the release of IFN-γ. We demonstrated that the decreased expression of the mature form of aminopeptidases cathepsins C and H, which regulate the activation of effector granzymes in NK cells, correlate with a lower cytotoxic function. Lower levels of mature cathepsins C and H can be a result of impaired processing from their precursor forms and their activity can be further decreased by a high level of monomeric, N-terminally truncated form of a cysteine protease inhibitor cystatin F, which co-localised with both enzymes in endosomal/lysosomal vesicles in NK cells.

The molecular neurodegeneration group has continued their work on the molecular processes involved in amyotrophic lateral sclerosis (ALS) and frontotemporal dementia (FTD). The main focus of the research is the RNA binding proteins TDP-43 and FUS as well as the newly discovered mutation in the C9orf72. Regarding TDP-43 and FUS, we did follow-up studies on their effects on the transcriptome. We also started the analysis of the stress-related changes in transcriptional and translational fidelity of these two genes. We have started a collaboration with prof. Plavec at the National Institute of Chemistry Slovenia to analyse the structure of the GGGGCC repeat using NMR and CD and are using RNA pull-down techniques to discover the proteins that bind G4C2.

We have finalized the work on the RNA binding properties of FUS (fused in sarcoma) and the effect on splicing and RNA processing. The study showed that FUS binds along the whole length of the nascent RNA with a limited sequence specificity to GGU and related motifs and increased crosslinking of the FUS in introns around the repressed exons. We have also reported on the deleterious effect of wild-type FUS overexpressed in transgenic mice and analysed the involvement of Transportin 1 in the nuclear transport of FUS in ALS. Furthermore, we continued the analysis of the newly discovered mutation in the C9orf72 gene and showed that the mutation has a single founder and is the most common mutation in familial and sporadic ALS in Europe and further characterised the expression of p62 as a major marker for ALS/ utation. Additionally we have written a review article on exploiting microP.

FTLD associated with C9orf72 gene mutation. Additionally, we have written a review article on exploiting microR-NAs for cell engineering and therapy. For World ALS Day (21 June 2012) Dr Rogelj had a guest lecture entitled New discoveries in ALS research, organized by the Dystrophy Society of Slovenia.

In the field of research of lactic acid bacteria, we improved the surface display on *Lactococcus lactis* with the use of BmpA as a carrier protein. A truncated version of BmpA, designated Bmp1, has increased the surface display ability by 3.3-fold. At the same time, we established that the over-

expression of BmpA on the bacterial surface increased the ability of bacteria to adhere to the Caco-2 epithelial cell model. This increases the usefulness of this technology in intestinal delivery applications.

We have successfully displayed several model binding proteins from the group of DARPins on the bacterial surface and confirmed their functionality. DARPins are antibody mimetics, obtained with genetic engineering on the basis of ankyrin repeats. We have demonstrated that two different DARPins,

Figure 2: Macrocypins, protease inhibitors from fungi have a negative effect on the growth and development of Colorado potato beetle larvae.

Transgenic mice overexpressing wild-type human FUS develop an aggressive phenotype of amyotrophic lateral sclerosis.

The role of cystatin F in the regulation of NK cell cytotoxicity was demonstrated.

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with either two or three ankyrin repeats, are both capable of binding the Fc region of human immunoglobulin.

We have successfully expressed the recombinant non-toxic subunit of the shiga toxin, StxB, purified it and determined the appropriate folding conditions. The functionality of StxB was confirmed by its specific binding to the Gb3 target receptor. The shiga toxin subunit will be used as a target for the development of binding proteins. These will be appropriate for the display on lactic acid bacteria, with the goal of treating the infections in which the shiga toxin is released (Shigella, ETEC).

We have expressed, in *L. lactis*, an infra-red fluorescent protein (IRFP) that enables the tracking of the bacteria with the use of infra-red light. This will enable monitoring of bacteria in vivo in animal models, as the light in infra-red region penetrates deeper into the tissue.

In our continuing study on plant responses to drought, a serine endopeptidase from common bean (Phaseolus vulgaris), was isolated and characterised at the protein level. Termed PvSLP2, its complete gene and

cDNA sequences were determined. A second endopeptidase, PvSLP1, was identified at the gene level, using primers based on the gene sequence of the putative drought-induced serine protease from Arachis hypogaea. The deduced amino acid sequences of these two previously unknown proteases are characteristic of those of plant subtilases of

the S8 family of clan SB. The sequence identity between them is only 33 %. The withdrawal of water had no effect on the expression of the transcripts of either protease, but the PvSLP2 proteolytic activity in leaves increased, to a degree depending on the age and position of the leaf. These results point to the regulation of PvSLP2 subtilase activity at translational and/or posttranslational levels and suggest a specific role in the response to drought

and senescence. The presence of several serine endo- and aminopeptidases was demonstrated in leaves of model plants Ramonda serbica that had been kept in a state of complete desiccation for 18 months. The plants could be revived by re-watering, when the activities of these proteases decreased.

The results of the research work at the Department of Biotechnology in 2011 were published in 36 scientific papers in journals with an impact factor, in a book and in eight chapters in books and presented in scientific conferences as lectures and posters. The members of the department were also very active in pedagogical work as lecturers and mentors to students preparing diploma and doctoral thesis at universities in Slovenia and abroad. Figure 4. Co-localisation of cathepsin C and cystatin F in NK cells.

Some outstanding publications in the past year

- Bratkovič, T., Glavan, G., Štrukelj, B., Živin, M., Rogelj, B.: Exploiting microRNAs for cell engineering and 1. therapy, 2012, vol. 30, issue 3, pp. 753-765. [COBISS.SI-ID 3197041], IF 9,7
- Mitchell, J. C., Rogelj, B., and assoc.: Overexpression of human wild-type FUS causes progressive motor neuron 2. degeneration in an age- and dose-dependent fashion. Acta Neuropathol, [in press] 2012, 16, doi: 10.1007/ s00401-012-1043-z. [COBISS.SI-ID 26073127], IF 9,6, A
- Erjavec, J., Kos, J., Ravnikar, M., Dreo, T., Sabotič, J.: Proteins of higher fungi from forest to application. 3. Trends biotechnol. (Regul. ed.). [Print ed.], 2012, vol. 30, issue 5, pp. 259-273. [COBISS.SI-ID 2504527], IF 9,2

INTERNATIONAL PROJECTS

- 1. ALSTransfid: Stress TDP43 Does stress induced reduction of translation fidelty play a role in ALS/FTLD? Fondation Thierry Latran
- Prof. Boris Rogelj
- 2 Bioactive substances in endemo-relict plants of the Balkan peninsula Slovenian Research Agency Prof. Janko Kos

RESEARCH PROGRAM

Pharmaceutical biotechnology: Knowledge for health Prof. Janko Kos



Figure 3: The use of micocypis as ligands in affinity chromatography on monoliths as solid support.

36 scientific papers in journals with an impact factor were published in 2012. An international patent application was also filed.



R & D GRANTS AND CONTRACTS

- Expression and functional analysis of non-coding RNA in Parkinson disease 1. Prof. Boris Rogelj
- 2 Functional analysis of proteins resistant to drought and insects Dr. Ierica Sabotič
- 3. Response to water stress in common bean (Phaseolus vulgaris L.): Proteomic analysis and QTL mapping Prof. Janko Kos
- Transport and RNA binding of TDP-43 and FUS implications for ALS/FTLD spectrum of neurodegenerative disease
- Prof. Boris Rogelj 5. Inhibitors of cysteine carboxypeptidases as regulators of autoimmune and neurodegenerative processes Prof. Janko Kos
- Regulation of T-cell functions with alpha type 1-polarised (alphaDC1) and standard 6 dendritic cells (sDC) Asst. Prof. Nataša Obermajer

VISITORS FROM ABROAD

1. Miguel Lozano Alonso, Centro para la Calidad de los Alimentos (INIA), Soria, Spain, 13. 1.-3. 4. 2012

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- 1. Prof. Kristina Gruden*
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- 7. Asst. Prof. Nataša Obermajer, left 01.05.12
- 8. Dr. Jure Pohleven
- 9. Dr. Jerica Sabotič

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- Dr. Sabina Vatovec
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- Slavko Kralj, Functionalization of magnetic nanoparticles for biomedical applications: doctoral dissertation, Ljubljana, 2012 (mentor Darko Makovec; co-mentor Janko Kos).
- 4. Špela Magister, *Regulation of cysteine proteases by inhibitor cystatin F in immune cells:* doctoral dissertation, Ljubljana, 2012 (mentor Janko Kos).
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- Marko Petek, Interactions between potato (Solanum tuberosum L.), potato virus Y (PVY) and Colorado potato beetle (Leptinotarsa decemlineata Say) at molecular level: doctoral dissertation, Ljubljana, 2012 (mentor Kristina Gruden).
- Matija Rojnik, *The role of cathepsin H in human cells:* doctoral dissertation, Ljubljana, 2012 (mentor Janko Kos).

DEPARTMENT OF ENVIRONMENTAL n-2SCIENCES

The activities in the Department of Environmental Sciences are as diverse and varied as the environment itself. They are multidisciplinary, ranging from various natural sciences to social sciences, in particular, chemical, physical, geological and biological, which define our environment, society, and human activities. With our research work we want to clarify the relationship between natural processes and human activities, and the influence of these activities on human health and the environment. The scope of our studies, the educational and technological aspects of research and development are thematically described in the following sections: Environmental analytical chemistry, Biological and geochemical cycles, Environment, nutrition, health, Environmental monitoring, Clean technologies and waste management, Risk and environmental impact assessment. The research summaries and the outline of activities of the research groups and centres within the Department of Environmental Sciences are presented in these sections.



Environmental analytical chemistry

Environmental analytical chemistry in the analytical laboratories and infrastructure centre for mass spec- Prof. Milena Horvat trometry, which operates as part of the Department of Environmental Sciences, carried out isotope geochemistry, radiochemistry and trace analysis in the field of organic and inorganic analysis.

In the field of the analysis of organic compounds we have devoted most of our research to studying the fate of pharmaceutical residues and endocrine-disrupting compounds. In addition to the representatives of non-steroidal anti-inflammatory drugs, lipid regulators, hormones, tranquilisers and antidepressants already investigated, we introduced a series of analytical procedures for determining cytostatics and industrial compounds with endocrine disrupting effect.

In the area of cytostatic research within the framework of FP7 CYTOTHREAT we have developed analytical procedures for determining selected compounds (5-fluorouracil, capecitabine, cyclophosphamide, ifosfamide) in environmental concentrations (ng/L). We have also studied their presence in hospital and municipal wastewaters

as well as receiving surface waters. We have shown the presence of detectable quantities of studied compounds mostly in wastewaters from hospitals where cancer therapy with selected compounds is being conducted. Some representatives have also been determined in municipal wastewater treatment plant influents. We also studied the bio- and photodegradation of fluorouracil and capecitabine and are the first to identify a number of their transformation products formed during these processes. In the area of endocrine disrupting compounds, we devoted research to industrial chemicals and personal care product ingredients like bisphenol A, triclosan, parabens and benzophenones. The first three compounds we developed within the framework of the FP7 DEMOCHOPHES project analytical procedure for their determination in urine samples. We have also analysed over 250 samples from human biomonitoring performed within this EU project. For benzophenones, which are structurally a common denominator for UV filters and selected pharmaceuticals, we have developed analytical procedures for their determination in environmental samples (aqueous and sediment samples). We have also begun to research their cycling in the environment.

Methods of isolation and analysis of isotopic composition of light elements in individual proteins in dairy and fruit products, used for a determina-



Figure 1: Correlation between daily mean values of radon concentration (\check{C}_{Rn}^{GC}) and [CO2] at Gaily Coloured Corridor (GC) location depending on the outside air temperature (colour scale)

tion of their geographic origin and the detection of adulteration were optimised. Methods for determining the isotope composition of lipids and polycyclic aromatic hydrocarbons (PAH) were applied in studies of the decomposition of organic matter in different environments, while molecular and isotopic analyses of PAH were used for tracing sources of contamination. The remains of food in archaeological samples of ceramics were studied using molecular and isotopic analyses of fatty acids and di- and triglycerides using ESI Q-TOF MS and ESI Q-TOF MS/MS.

In radiological chemistry three different dissolution techniques were tested for the determination of ²¹⁰Po in biological samples. The dissolution techniques involved the classic wet ashing with acids by heating vigorously over

a gas flame, the digestion with acids up to 200°C and the wet digestion by a microwave system in Teflon vessels. The results obtained revealed that the activity concentrations of ²¹⁰Po found in biological samples were not statistically different among the three applied approaches.

Three different dissolution techniques for the determination of uranium in soil were compared: the conventional total dissolution with mixtures of acids; the microwave dissolution using acids; and the alkaline fusion. The results obtained showed that the best dissolution was achieved with alkaline fusion. As a measurable amount of uranium was found in the residue after digestion with the two commonly used dissolution techniques, further investigations are required.

In the area of chemical metrology the department collaborated on the international project ERMP ENVO2 PartEmission (Emerging Requirements for Measuring Pollutants from Automotive Exhaust Emissions) where it leads and coordinates Workpackage 4 (WP-4). The goal of WP-4 is to provide traceable and accurate mercury calibration standards and improved and validated measurement techniques, which will meet modern needs in analytical chemistry. In the scope of WP-4, we successfully concluded task 4.1 which included the evaluation and testing of mercury-resistant materials for low-level Hg sampling in collaboration with VSL, The Netherlands.

In the area of chemical metrology two types of activities need to be mentioned. The first is related to the certification of trace elements in candidate Certified Reference Materials for the EU, JRC, Institute for Reference Materials and measurements (IRMM): (i) ERM-EF411 hard coal, ERM-EF412 brown coal and ERM-EF413 furnace cake for As, Co, Cr, Hg, Mn, Sb, Se, V, Zn, Ca, Mg, Na, K and Cl, (ii) ERM-BD150 and ERM-BD151 Skimmed milk for Ca, Cl, Co, Fe, K, Mg, Mn, Na, Se and Zn and (iii) Ag in Chicken paste and Ag suspension. In addition, a series of CCQM Key Intercomparisons were also organized. Based on the excellent performance a series of CMC (Calibration Measurement Capability) claims are planned for 2013, which will be later entered in the KCDB (Key Comparisons Data Base). Furthermore, ordinarily participation in inter-laboratory comparison studies organised by IAEA, WEPAL and others reference laboratories is our mission, as well as their organization.

Centre for Mass Spectrometry participates in research and application projects with mass spectrometric measurements on high resolution tandem mass spectrometer Q-Tof Premier, equipped with electrospray ionization source (ESI), which is also coupled with ultra-performance liquid chromatograph (UPLC). This instrument was used for the identification and quantification of Ni complexes with quinic acid in different sorts of tea, accurate detection of Zn citrate in milk and analysis of traces of di-and tri-acylglicerides in archaeological samples of vessels for cooking or food storage. Some transformation products of drug benzodiazepine and their influence into environment were determined with LC-MS.

Biological and geochemical cycles

The natural distribution of elements in the environment determine the isotopic composition of these substances in air, water, soils and allow monitoring of the biological and geological cycles and measuring their impact on organisms.

In the framework of the EU 7OP GMOS project, Global Mercury Observing System, aiming at establishing a global monitoring infrastructure for the Hg measurements in the air two important activities were accomplished. In cooperation with the GMOS consortium and GEOTRACES network co-workers participated in a sampling expedition along 40th parallel in the South Atlantic Ocean on the research vessel RSS James Cook. Results of this expedition are first high resolution spatial results obtained along this stretch of the South Atlantic. The results are important because a considerable part of biological production is concentrated along the 40°S, which has substantial influence on the cycling of the elements in the ocean, including Hg. We also joined a research cruise on board the Italian research vessel Urania, where we studied the cycling of different Hg species in a marine environment. The cruise was a continuation of the work done within previous EU projects (MEDOCEANEOR, MERCYMS, etc.). We measured the concentrations of different Hg species in a water column at 13 locations of the Western Mediterranean and Atlantic part of the Strait of Gibraltar, which is of crucial importance for understanding the element exchange between the Mediterranean and the Atlantic Ocean.

In collaboration with the Slovenian Environmental Agency (ARSO) we monitored the concentrations of total Hg in precipitations and gaseous Hg in air at international meteorological station in Iskrba near Kočevska Reka. In past year we installed a Tekran system that allows measurements of different Hg species in air (gaseous oxidized Hg – GOM, gaseous elemental Hg – GEM, particulate bounded Hg – PBM and total gaseous Hg – TGM), which will improve our understanding of the cycling and sources of Hg in the local and global environments, and a comparison of different measurement techniques.

In the group of geochemistry the contribution of natural processes to the carbon mass balance of Slovenia was analysed. The biogeochemical cycle of carbon is tightly coupled to the hydrological cycle and biogeochemical cycles of other elements, in particular nutrients. Different environments were studied, among others the weathering and dissolution of bedrock, primary and secondary precipitation in water, back-precipitation within aquifers, decom-

position of organic matter in the water column and in sediments, in the soil and processes within coal seams. The origin of particulate organic matter in the water column and the seasonal dynamics of the primary production and mineralization of alochtonous and autochtonous organic matter in Lake of Bled were investigated.

Stable isotope analyses of carbon in methane, bulk sedimentary organic matter and in lipids, as well as their molecular composition, were used to support the terminal restriction fragment length polymorphism (T-RFLP) analysis of 16S ribosomal ribonucleic acid (rRNA) sequences of bacterial and archaeal community members and confirmed that larger sediment-depthdependent changes occurred in the latter. The detected biogeochemical processes and structure of the archaeal community supported the hypothesis that hydrogenotrophic methanogenesis is the dominant pathway in the sediment, despite the low temperature and the prevalence of "fresh" autochthonous-derived organic matter. In contrast to hypoxic and anoxic lacustrine environments, methanogenesis in coal seams proceeds by the microbial CO₂ reduction, which was confirmed by the carbon stable isotope analyses of methane, carbonate host rock and the highly alkaline water in the Velenje coal basin.

Seasonal variations in the concentration and sources of CO₂ in the soil atmosphere at abandoned pasture and meadows in the Podgorje Kras area were investigated. It was shown that, on an annual basis, the bedrock weathering contributes a comparable amount of CO₂ as respiration and decomposition of soil organic matter.

Research on carbon cycling in Slovenian river catchments was extended to Alpine springs. The age of the water in the springs was determined by the ³H activity and was on average between 2.6 and 5 years. The source of dissolved inorganic carbon, which is reflected in its carbon stable isotope composition, was shown to be a reliable indicator of the vulnerability of the spring catchment area to anthropogenic pollution.

A multivariate statistical data evaluation was used to evaluate the results of the long-term monitoring of the hydrochemical and isotopic composition of water in Krka River (Croatia), where geogenic and anthropogenic contaminants were discriminated.

In the radiochemistry group the fractionation of the natural radionuclides in the soil and fresh water sediments as well as the transport of natural radionuclides into the biological systems and food chain were investigated. The transfer of uranium-radium decay chain radionuclides from hay and silage to cow's milk were assessed in the vicinity of the former uranium mine and mill Žirovski Vrh. The knowledge of site-specific transfer factors is required for assessing the radiation doses to the population. The sedimentation Figure 2: Iso-concentration areas of a) 40K, b) 232Th, and c) 226Ra in rate in the Middle and South Adriatic Sea was assessed by the measurement of 137Cs activity concentrations in the sediment profiles. The rate was found to be between 1.8 and 4 mm y^{-1} .



soil at 70 points in Slovenia

¹²⁹I is important as an environmental tracer of the biogeochemical cycling of iodine and of the dissemination of nuclear pollution, because anthropogenic ¹²⁹I has been released from only a few point sources and with its short mixing time its distribution therefore reveals the movement of ¹²⁹I in the environment. The RNAA was applied to determine ¹²⁹I/¹²⁷I isotopic ratios as well as ¹²⁹I and ¹²⁷I concentrations in soils from several locations in Ukraine and from Slovenia. The ¹²⁷I concentrations in surface soils from Ukraine were in the range 2.3-23.1 µg g⁻¹ and for 129 I (11.1-245.7) \cdot 10⁸ µg g⁻¹ dry matter with the highest value of 1.47 \cdot 10³ µg g⁻¹. In soil samples from Slovenia 127 I $concentrations\ ranged\ 0.73-130\ \mu g\ g^{\scriptscriptstyle 1}\ and\ ^{\scriptscriptstyle 129}I\ (8.0-245.7)\cdot 10^{\scriptscriptstyle 8}\ \mu g\ g^{\scriptscriptstyle 1}.\ The\ ^{\scriptscriptstyle 129}I/^{\scriptscriptstyle 127}I\ isotopic\ ratios\ of\ the\ surface\ soils\ rate of\ the\ surface\ soils\ rate of\ rate of$ from Ukraine were in the range of the order of 10⁹-10⁵ and of 10⁻¹⁰-10⁻⁸ for the soils from Slovenia.

One of the studies in Centre of radon was the dependence of radon levels in the air of karst caves on atmospheric and geophysical parameters was mainly oriented to the influence of microclimatic and geomorphological characteristics on the spatial distribution of radon levels in Postojna Cave. The direction of air flows and the extent of ventilation were studied on the basis of continuous measurements of radon concentration at three measurement locations, which was found very useful for the interpretation of the results of nano aerosol measurements in Postojna Cave. We have been focused on the role of the concentration and size distribution of the background (non-radioactive) nano aerosols on the size distribution of nano particles of radon decay products (especially the <10 nm fraction), the presence of microorganisms in the cave air (Karst Research Institute, Research Centre of the Slovenian Academy of Sciences and Arts), and the influence of the tourist visits on the nano aerosol behaviour. In the frame of the FP 7 project BlackSeaHazNet the research of the effects of seismic activity and tectonic faults on radon levels has been continued. The transport of radon and carbon dioxide has been studied in soil gas on different geological bedrocks in Slovenia and Japan (the Japanese–Slovenian bilateral project), and radon and thorium in the air of living environment within bilateral projects with Hungary and Serbia.

Environment, nutrition, health

Numerous researches and measurements of various environmental parameters, food and health effects of pollutants are among the major activities at the Department of Environmental Sciences.

Two EU projects COPHES and DEMOCOPHES were finished after 3 years of work. They both together have demonstrated that a more coordinated and harmonised approach to human biomonitoring (HBM) in Europe



Figure 3: The analysis and speciation of mercury was made on the Research vessel James Cook in the South Atlantic as part of the GEOTRACES and GMOS projects. A significant decrease of dissolved gaseous mercury in the surface waters was observed. The evasion of mercury from the ocean surface represents the largest natural source of mercury to the global atmosphere.

is possible and also useful to protect the health of Europeans. For the first time we have results which are comparable across Europe. Biomarkers for chemicals of concern were measured in the hair and urine of almost 4000 mothers and their children in 17 European countries. Mercury was measured in hair and cadmium, cotinine, phthalate metabolites, bisphenol A, triclosan and parabens were analysed in urine. Europe is not homogeneous; differences in the levels were seen between the countries, indicating that there are differences in exposures. Many of the differences may be explained by lifestyle or differences in diet.

We also studied the transfer of toxic elements from mother to child though breast feeding using a classic analysis of trace elements in human milk and the use of the deuterium method standardised by the IAEA. The method has been applied in Slovenia for the first time.

The distribution and speciation of selenium (Se) in freshwater fish (muscle and liver tissue) from lakes in Argentina was investigated. Values for total Se in muscle ranged from $0.66 \,\mu\text{g/g}$ to $1.61 \,\mu\text{g/g}$, while in the liver the concentrations were much higher, from $4.46 \,\mu\text{g/g}$ to $73.71 \,\mu\text{g/g}$ on a dry matter basis. The separation of soluble Se species was achieved by ion-exchange chromatography, and detection performed by ICP – MS. The results showed that in fish muscle from 47 to $55 \,\%$ of selenium was soluble

and the only Se species identified was SeMet, which represented around 80 % of the soluble Se, while in the liver the amount of soluble Se ranged from 61 to 76 % and the percentage of species identified (SeMet and SeCys2) ranged from 8 to 17 % of soluble Se.

In the context of the CRP project, whose objective is to monitor the quality of the fish on the Slovenian market, we analysed the content of essential and toxic elements in two groups of fish (Atlantic salmon, trout and European seabass from fish farms and wild fisheries). The levels of the toxic elements As, Cd and Pb are comparable with those in the literature, the concentrations of Cd and Pb are below the limit of detection for the method used (<3ng/g and <23 ng/g dry weight). The content of the essential elements Fe, Zn and Cu is not significantly different between the farmed and wild seabass, while the element contents are higher in the sea than freshwater fish.

MT mRNA expression was studied in human glioblastoma cell line U87 MG (American Type Culture Collection, USA) before and after the arsenic trioxide exposure. The gene expression of six metallothionein (MT) (sub) isoforms, namely MT2a, MT1 (a, e, f, x) and MT3, was followed by qPCR. The cells were treated by arsenic with or without vitamin C addition. Suppressed expression was observed after exposure to a low concentration and increased expression after exposure to higher concentrations, especially for the isoforms MT1 (f, x) and MT2a. Both phenomena were tested by cadmium and mercury exposure. The results are interesting regarding chemoresistance during cancer treatment and as resistance against the toxic effects of metals present in food and water or in the working environment (occupational exposure). Next to biomedical research we also studied the arsenic in marine environment and food. In muscle samples of the Mediterranean ray high concentrations of non-toxic arsenobetaine were found while liver samples also contained dimethylarsinic acid and traces of inorganic arsenic. There are little data on arsenic speciation in ray samples and other Cartilagineous fish and our study shows similarities in the arsenic speciation with better known and more common bony fish. In the terrestrial environment we modelled the arsenate behaviour in soil and studied the accumulation, distribution and speciation of arsenic in desert plant Atriplex atacamensis, grown wild in arsenic polluted arid areas of Chile. We demonstrated that the combination of a multi-element analysis, several isotopic ratios (^{13}C / ^{12}C , ^{15}N / ^{14}N , ^{18}O / ^{16}O , ^{2}H / ^{1}H) and selected chemical and physical parameters (fruit mass, antioxidant activity, content of ascorbic acid and total phenols) can be used to differentiate the varieties of Slovenian apples, the geographical location of their growth and agricultural practice. The botanical origin (cultivar) was found to have a major influence on the δ 13C and δ 15N values of the proteins and the $\delta^{18}O$ and δD values of the water. The geographical regions were well separated based on the $\delta^{18}O$ and δD values in the water and the concentrations of Rb and S in fruit juice. The most significant variables to distinguish between the organically and conventionally cultivated fruits were found to be the 15N/ 14N ratio and the anti-oxidant activity. In addition, significant differences were also observed in the ascorbic acid content.

Stable isotopes of nitrogen were also used to estimate the risk of nitrate leaching into the groundwater during lettuce production using different irrigation and fertilities practices. Broadcast application combined with irrigation was identified to provide the optimal yield at minimum risk for the groundwater quality.

With the radiochemistry methods the activity concentrations of natural radionuclides ²¹⁰Po and ²¹⁰Pb in edible Mediterranean mussels from the Adriatic Sea were determined. Both radiotoxic nuclides are decay products of the same parent. Nevertheless, the activity concentrations of ²¹⁰Po in organisms were 6.2 to 30.7 higher than the activity concentrations of ²¹⁰Pb, thus indicating their different biological role in organisms.

In the group of inorganic analytical chemistry the monolithic chromatography is frequently used in speciation analysis. An analytical procedure that includes the use of convective-interaction media (CIM DEAE-1) column coupled to inductively coupled plasma mass spectrometry (ICP-MS) was applied in investigations on the kinetics, binding and distribution of chemotherapeutics based on platinum or ruthenium in human serum samples. One CIM Protein G and one CIM DEAE disks were assembled together in a single housing forming CLC monolithic column. Such a set-up allows rapid twodimensional separation, by affinity and ion-exchange modes, to be carried out in a single chromatographic run. A complex investigation was carried out in order to develop an analytical method for a quantitative determination of Zn-citrate in human milk samples.

In addition to monoliths, stable isotopes were also included to the speciation analysis. The application of a high matrix introduction system, high-energy collision mode and careful optimisation of the ICP parameters enabled the efficient reduction of polyatomic interferences of chlorine and carbon ions in the determination of chromium at m/z 52 and 53. This al-



Figure 4: Typical chromatogram for the separation of Se species in the extract of fish liver, on cation exchange (Zorbax 300-SCX column).

lows us to use previously properly synthesized chromium species (${}^{50}Cr(VI)$ and ${}^{53}Cr(III)$) either as tracers of species transformation during the analytical procedures applied and for quantification of the Cr(VI) by isotope dilution ICP-MS technique. Such an analytical methodology was successfully applied for a highly accurate determination of Cr(VI) in corrosion-protection coatings.

On the field of organotin compounds research, stable isotope labelled tri- and di-butyl species were laboratory synthesized and surveillance monitoring of the pollution along the Croatian part of the Adriatic Sea carried out. Inter-institutional collaboration in multidisciplinary teams that carried out complex studies ended up in successful synthesis of the surface-modified magnetic nanoparticles that were applied for effective immuno-gene therapy of murine mammary adenocarcinoma. Finally, in collaboration with University of Padova, the effects of a copper-deficient diet in aged CD1 mice and the influence of such a diet on the main organs and in different brain areas were investigated.

Environmental Monitoring

Research groups of the Department of Environmental Sciences performed regular and long-term measurements of various environmental parameters to control potential contaminations exposure to pollutants in the environment.

In collaboration with the Chemical Office of the Republic of Slovenia, University Medical Centre Ljubljana, regional institutes of Public Health, regional hospitals and health we continued national human biomonitoring. We analyse toxic chemicals including toxic metals (cadmium, lead, mercury) and persistent organic pollutant including dioxins, pesticides, PCBs, polybrominated flame retardant in human blood, urine and maternal milk. The results will be used for the assessment of the burden of the Slovenian population with these environmental pollutants.

With isotopic analyses the monitoring of a stable isotope composition of precipitation and surface water in Slovenia was continued. The database of isotope parameters of wine in line with EU requirements was upgraded, as well as the database on the isotope composition of the coal bed gases in the Velenje Coal Basin.

The monitoring of the carbon isotope composition in the environment close to the NPP Krško was upgraded with the first data on stable carbon isotopes in plants in the surroundings of the power plant.

The monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski Vrh was performed.

In collaboration with the Environmental Agency of the Republic of Slovenia the monitoring of organotin compounds in surface and sea water was continued in 2012.

The Department of Environmental Sciences also organised the mobile chemical laboratory ELME for intervention in the case of environmental accidents with hazardous materials. The chemical mobile unit had four interventions in 2012 as a result of environmental pollution.

Clean technologies and waste management

The activities of the Department of Environmental Sciences are closely linked to the introduction of cleaner, more environmentally friendly technologies and waste management.

In collaboration with the Department of Inorganic Chemistry and technology we continued our research on cost-effective methodologies for the removal of mercury in flue gases by the oxidation method in flue-gas desulfurization plants. Mathematical models were introduced and used for the simulation of aqueous Hg chemistry. Mercury behaviour in solid samples at higher temperatures was also studied as part of the initial experiments of the removal of Hg from gases at higher temperatures.

In collaboration with the Faculty for Civil Engineering and the Faculty for Mechanical Engineering, University of Ljubljana we have studied the removal of organic pollutant residues from wastewaters by hydrodynamic cavitation. An optimised process was coupled to biological wastewater treatment and UV degradation.

In collaboration with the Biotechnical Faculty, University of Ljubljana, a study was made of the influence of selected new emerging contaminants on the development of biomass during wastewater treatment.

In the field of nanotechnology we developed an analytical method for the one-step synthesis of a thin layer of TiO_2 on Ti_6Al_4V alloy for the improvement of short-term and long-term body responses. This method decreases the direct contact between the bone tissue and metals, especially aluminium and vanadium, and improves bone-tissue integration.

Risk and environmental impact assessment

People are exposed to a large number of pollutants in the environment, but the exposure is relatively difficult to evaluate, especially when it comes to long-term exposure to low levels of pollutants. Therefore, an accurate assessment of exposure is very important in order to estimate the correct risk assessment.

The approach to the sustainability appraisal of nuclear energy in Slovenia (Krško) has been developed as a basis for long-term national energy-policy approval. The EU project iNTeg-Risk was a framework for making guidelines for the integration of strategic, sustainability and project-level impact evaluation with land-use planning for new and emerging risk technologies. The CIVITAS ELAN project has been successfully concluded as well as Targeted Research Project on strategic environmental assessment (SEA) in Slovenia. One of the results of the latter is a CBA for the two formal SEA procedures: one for a highway section around Škofljica and the other for the strategic spatial plan for the Municipality of Ljubljana.

The annual ingestion dose due to milk consumption for the natural radionuclides influential area of the former uranium mine and mill at Žirovski Vrh was assessed. The estimated dose is low, with the highest contribution due to ²¹⁰Po in ²¹⁰Pb. The ERICA Tool was applied for an assessment of the radiation impact on some terrestrial and aquatic organisms from the Žirovski Vrh area. The assessed dose rates were low, being in the range from several to tenths of μ Gy h⁻¹. Within the EMRAS II project coordinated by the International Atomic Energy Agency, the department's staff participated in the inter-comparison of modelling approaches for assessing doses to terrestrial wildlife.

In the frame of EU 7FP EGIDA (Coordinating Earth and Environmental cross-disciplinary projects to promote GEOSS) project that ended in 2012, the EGIDA methodology developed within the project was evaluated at the level of Slovenia. The methodology aims to provide support to the promotion and coordination of activities carried out by: the GEO Science & Technology (S&T) Committee; S&T national and European initiatives; and other S&T Communities.

We participated in the preparation of the new global convention on mercury, coordinated by the United Nations Environment Programme (UNEP). Background documents were prepared which comprise four main chapters: atmospheric emissions, Hg entering the aquatic environment; and the fate and transport of mercury in the atmosphere and in aquatic environments. Our main responsibility was the preparation of the chapter dealing with releases of Hg into aquatic ecosystems from a variety of anthropogenic and natural sources, which represents the first calculation at the global level.

Some outstanding achievements

- 1. In the framework of the new Global mercury Convention to be adopted in 2013, a report on mercury releases to the aquatic systems at the global level was prepared for the UNEP Secretariat. This forms an integral part of the new UNEPs Global Mercury Assessment 2012 report, which represents an essential part in the on-going negotiation process.
- 2. We studied bio- and photodegradation of cytostatic drugs fluorouracil and capecitabine and are the first to identify a number of their transformation products formed during these processes.
- 3. In the group of inorganic analytical chemistry developed new methods based on monolithic chromatography. An analytical procedure that includes the use of a convective-interaction media (CIM DEAE-1) column coupled to inductively coupled plasma mass spectrometry (ICP-MS) was applied in investigations on kinetics, binding and the distribution of chemotherapeutics based on platinum or ruthenium in human serum samples.
- 4. The reason for an order of magnitude higher radon concentration in summer time in the Gaily Coloured Corridor than in other parts of the Postojna Cave was clarified in Centre for Radon.
- 5. In two EU projects COPHES and DEMOCOPHES comparable results have been obtained in 17 European countries on the exposure of children and their mothers to mercury, cadmium, cotinine, phthalates, bisphenol A, triclosan and parabens. Differences in exposure can be explained by lifestyle or differences in diet.
- 6. A method for comprehensive cost-benefit analysis (CBA) related to SEA procedure in Slovenia has been developed and tested on two cases.
- 7. An integrated impact assessment of sixteen traffic improvement measures in Ljubljana has been made in the framework of the CIVITAS Elan project including CBA for five selected measures.
- 8. Development, testing, and validation of the integrated, hierarchically consolidated methodology for the evaluation of sustainability, environmental risks and land-use planning for new hazardous installations have been made in the framework of the iNTeg-Risk project.

Some outstanding publications in the past year

- 1. Novotnik, B., Zuliani, T., Ščančar, J., Milačič, R.: The determination of Cr(VI) in corrosion protection coatings by speciated isotope dilution ICP-MS. J. Anal. At. Spectrom., 2012, 27(9), pp. 1484–1493
- 2. Mulec J., Vaupotič J., Walochnik J.: Prokaryotic and eukaryotic airborne microorganisms as tracers of microclimatic changes in the underground (Postojna Cave, Slovenia). Microb. Ecol., 2012, 64(3), pp. 654-667
- 3. Mechora, Š., Germ, M., Stibilj, V.: Selenium and its species in the aquatic moss Fontinalis antipyretica. Sci. total environ., 2012, 438, pp. 122–126
- 4. Mandić-Mulec, I., Gorenc, K., Petrišič, M. G., Faganeli, J., Ogrinc, N.: Methanogenesis pathways in a stratified eutrophic alpine lake (Lake Bled, Slovenia). Limnology and Oceanography, 2012, 57(3), pp. 868–880
- Hines, M. E., Poitras, E. N., Covelli, S., Faganeli, J., Emili, A., Žižek, S., Horvat, M.: Mercury methylation and demethylation in Hg-contaminated lagoon sediments (Marano & Grado Lagoons, Italy). Estuar., coast. shelf sci., 2012, 113, 10, pp. 85–95
- 6. Kontić, B., Kontić, D.: A viewpoint on the approval context of strategic environmental assessments. Environ. impact. asses. rev., 2012, 32 (1), pp. 151–155

Awards and appointments

1. Radojko Jaćimović: awarded the degree of Honorary Doctor by Odessa National Polytechnic University, Ukraine, 23. 10. 2012

Organization of conferences, congresses and meetings

- 1. Milena Horvat: Workshop Mercury in contaminated sites: characterisation, impact and remediation, Ljubljana, Slovenia, 6.–8. 6. 2012
- Milena Horvat, Vekoslava Stibilj, Radojko Jaćimović, Tea Zuliani, Polona Vreča: Workshop on outcome of the Interlaboratory Comparison: Determination of Trace Elements in Sediment (PT- SED2), Ljubljana, Slovenia, 21. 11. 2012
- 3. Nives Ogrinc: scientific meeting Workshop on Assessment of Groundwater Resources Affected by Rivers in Danube Basin Slovenia, Ljubljana, 26.–29. 11. 2012

- 4. Ljudmila Benedik: Training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC Enlargement & Integration policy, Ljubljana, Slovenia, 27. 2. 2. 3. 2012, 16. 27. 4. 2012, 11. 22. 6. 2012, 3. 7. 9. 2012, 15. 26. 10. 2102
- 5. Mateja Bezek, Asta Gregorič, Janja Vaupotič: professional course Radon in buildings: measures to decrease radon concentrations, Jožef Stefan Institute, Ljubljana, Slovenia, 24.–25. 5. 2012

INTERNATIONAL PROJECTS

- 1. Provision of testing services for filter media used in IMS radionuclide stations CTBTO Preparatory Commission Prof. Ljudmila Benedik
- 7.FP CIVITAS-ELAN: Mobilising citizens for vital cities Ljubljana-Gent-Zagreb-Brno-Porto
 - European Commission Dr. Davor Kontić
- 3. 7. FP HYDRONET: Floating sensorised networked robots for water monitoring European Commission
- Prof. Milena Horvat
- 7. FP iNTeg-Risk: Early recognition, monitoring and integrated management of emerging, new technology related risks European Commission
- Prof. Branko Kontić
- 7. FP ArcRisk: Arctic health risks: Impacts on health in the arctic and europe owing to climate-induced changes in contaminant cycling European Commission
- Prof. Milena Horvat
- 6. FP COPHES: European coordinaton action on human biomonitoring European Commission
- Prof. Milena Horvat 7. FP - EGIDA: Coordinatir
- FP EGIDA: Coordinating Earth and environmental cross-disciplinary projects to promote GEOSS European Commission
 - Asst. Prof. Sonja Lojen
- 8. FP GMOS; Global mercury observation system European Commission
- Prof. Milena Horvat
- 7. FP CYTOTHREAT; Fate and effects of cytostatic pharmaceuticals in the environment and the identification of biomarkers for and improved risk assessment on environmental exposure European Commission
- Prof. Ester Heath
- 7. FP BlackSeaHazNet: Complex research of euarthquake's prediction possibilities, seismicity and climate change correlations European Commission
- Prof. Jania Vaupotič
- 7. FP CITI-SENSE: Development of sensor-based citizens' observatory community for improving quality of life in cities European Commission
- Prof. Milena Horvat
- 12. ACT CLEAN Access to technology and know-how in cleaner production in Central Europe
- European Commission
- Asst. Prof. Sonja Lojen 13. LIFE PLUS – DEMOCOPHES
- European Commission Prof. Milena Horvat
- 14. PartEmissio: EMRP Emerging requirements for measuring pollutants from automotive exhaust emissions
 - Euramet e.V.
- Prof. Milena Horvat
- EMRP: Traceable measurements for monitoring critical pollutants under the european water framework directive (WFD-2000/60/EC) Euramet e.V.
 - Prof. Radmila Milačič
- 16. Stable isotope technique to assess human milk intake in infants living in areas contaminated with mercury, lead and cadmium IAEA - International Atomic Energy Agency
 - Prof. Milena Horvat
- Stable isotopes in atmosphere-biosphere-earth system research (SIBAE) COST Office
- Asst. Prof. Sonja Lojen
- COST ES0801. The ocean chemistry of bioactive trace elements and paleoclimate proxies
 - COST Office
 - Prof. Nives Ogrinc
- 19. Use of Environmental isotopes in investigations of influence of snow melt on stream runoff in the area of Julian Alps, NW Slovenia

IAEA - International Atomic Energy Agency Dr. Polona Vreča

- 20. Assessment of human milk intake in infants living in gold mining areas in south west Nigeria, using stable isotope techniques IAEA - International Atomic Energy Agency
- IAEA International Atomic Energy Agency Dr. Darja Mazej
- Training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC enlargement and integration policy Institute for Reference Materials and Measurements Prof. Liudmila Benedik
- Characterisation of major and trace elements in three coal materials by activation and/ or destructive methods Institute for Reference Materials and Measurements
- Prof. Milena Horvat 23. Training fee for Ms Gulnura Abasova (Kyrgyzstan), TA00221759, 2. 2.- 1. 5. 2012 ICTP/IAEA Step Program, The Abdus Salam
 - Prof. Janja Vaupotič 4. Training fee for Ms Ilona Matveveva. (Kazakhstan). TA00221835
- Training fee for Ms Ilona Matveyeva, (Kazakhstan), TA00221835, 15. 2.-14. 5. 2012 ICTP/IAEA Step Program, The Abdus Salam Prof. Borut Smodiš
- 25. Stability monitoring of BCR-679 (only Hg Determination) and BCR-100 Institute for Reference Materials and Measurements Prof. Milena Horvat
- Characterisation of ERM-BD150 and ERM-BD151 skimmed milk Institute for Reference Materials and Measurements Prof. Milena Horvat
- Training fee for Ms Christiane Odumah Anderson, (Ghana), 1.10.–24. 12. 2012 ICTP - Centro Internazionale Di Fisica Teorica Prof. Milena Horvat
- Training fee for Ms Ilona Matveyeva, (Kazakhstan), 24. 9.–23. 12. 2012 ICTP - Centro Internazionale Di Fisica Teorica Prof. Borut Smodiš
- IAEA workshop /RER8016 9002/workshop on assessment of groundwater resources affected by rivers in Danube Basin, 26.–29. 11. 2012, Ljubljana, Slovenia IAEA - International Atomic Energy Agency Prof. Nives Ogrinc
- 30. SOP WHO Standard Operating Procedure World Health Organization Prof. Milena Horvat
- Determination of Ag in chicken paste and Ag suspension by k0-INAA Institute for Reference Materials and Measurements Dr. Radoiko Iaćimović
- Radojko Jacintović
 Determination of Ag in Ag suspension by k0-INAA Institute for Reference Materials and Measurements Dr. Radojko Jaćimović
- 33. Techno-economic evaluation of options for adapting nuclear and other energy infrastructure to long-term climate change and extreme weather IAEA - International Atomic Energy Agency Prof. Branko Kontić
- 34. Hydrogeochemistry of carbonate weathering fluxes at the terrestrial/marine interface of the Adriatic Sea: A collaborative field study Slovenian Research Agency
- Prof. Nives Ogrinc
- 35. Where is Radon (Gaseous Soil Component) coming from? Slovenian Research Agency Prof. Janja Vaupotič
- 36. Biogeochemistry of mercury in contaminated coastal environments; coastal lagoons in Rio Grande do Sul, Brazil and the Gulf of Trieste Northern Adriatic Slovenian Research Agency Prof. Milena Horvat
- Neutron activation analysis on the assessment of arsenic resistant plants from Santa Barbara Region, Iron Quadrangle, Brazil Slovenian Research Agency
- Dr. Radojko Jaćimović
- 38. Application of advanced methods in determination of geographic origin of wine: Comparison of Austrian and Slovenian wine Slovenian Research Agency Prof. Nives Ogrinc
- 39. Development of isotopic tools for better understanding of impacts of Sava and Danube

rivers on groundwater systems in Slovenia and Slovakia: better management of groundwater resources and their protection against contamination Slovenian Research Agency Prof. Nives Ogrinc

- Effect of short lived thoron progeny on effective dose at dwellings and workplaces in Slovenia and Hungary
 - Slovenian Research Agency Prof. Janja Vaupotič
- Mercury analysis and speciation in the oceans Slovenian Research Agency
- Prof. Milena Horvat
- 42. Fluid dynamics and carbon cycling in sedimentary basins: geochemical characterization, evaluation of biogeochemical processes and modeling Slovenian Research Agency Dr. Tiaša Kanduč
- Calibration of palaeoenvironmental records in (sub)recent laminated tufa Slovenian Research Agency Asst. Prof. Sonja Lojen
- Determination of toxicity and physico-chemical properties of pharmaceuticals Slovenian Research Agency Dr. Tina Kosjek
- Tracing of natural and anthropogenic impacts in marine ecosystem along Istrian Adriatic coast using mediterranean mussel *M. Galloprovincialis* Slovenian Research Agency Dr. Tiaša Kanduč
- 46. Environmental isotopes in snow hydrology Slovenian Research Agency
- Dr. Polona Vreča
- Mercury Processes in aquatic systems; mercury methylation and reduction in natural aquatic environments: laboratory studies using high specific activity 197Hg radiotracer Slovenian Research Agency Prof Milena Horvat
- Where is Radon (Gaseous Soil Component) coming from? Slovenian Research Agency Prof. Janja Vaupotič

RESEARCH PROGRAMS

- 1. Modelling and environmental impact assessment of processes and energy technologies Prof. Borut Smodiš
- Cycling of substances in the environment, mass balances, modelling of environmental processes and risk assessment Prof. Milena Horvat

R & D GRANTS AND CONTRACTS

- 1. The effect of selenium on the harvest and quality of crops Prof. Vekoslava Stibilj
- 2. Interaction of organic matter with metals in coastal waters of the Gulf of Trieste Prof. Milena Horvat
- Tartary buckwheat as a new source for functional foods Prof. Vekoslava Stibilj
- Synthesis, characterisation and use of novel ruthenium compounds in electrochemotherapy of tumors (basic research project) Prof. Janez Ščančar
- Sustainable land use in relation to soil and crop quality Prof. Nives Ogrinc
- Metagenomics for bioexploration and biomining of bacterial laccases for a sustainable environment Prof. Ester Heath
- Archaeologies of hunter-gatherers, farmers and metallurgists: Cultures, populations, palaeoeconomies and climate
- Prof. Nives Ogrinc 8. Advanced water treatment with ultrasound and cavitation Prof Ester Heath
- VISITORS FROM ABROAD
- Gulnura Abasova, Ministry of Health, Department of the State Sanitary and Epidemiological Surveillance, Bishkek, Kyrgyzstan, 2. 2.–30. 4. 2012
- Rossitza Borissova Karaivanova, Tsvetan Nedyalkov Piperov, State Enterprise for Radioactive Waste, Sofia, Bulgaria, 27. 2.–2.3. 2012
- Mihaela G. Bragea, Institute of Public Health, Timisoara, Romania, 27. 2.–2.3. 2012
- Martina Rožmarić Mačefat, Ruđer Bošković Institute, Zagreb, Croatia, 27. 2. -2.3. 2012
- 5. Bojan Šešlak, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 27. 2.–2.3. 2012

- The use of isotope dilution inductively coupled plasma mass spectrometry technique in environmental studies
- Prof. Radmila Milačič 10. Toxic metals and organometallic compounds in the terrestrial environment Prof. Radmila Milačič
- Speciation and interactions of chemical contaminants at trace level in aqueous media to support the development of cost-effective removal technologies Prof. Milena Horvat
- 12. Climate change and impacts of anthropogenic disturbances on primary production in forest soil
- Prof. Nives Ogrinc13. The impact of climate change on the sustainability, stability and biodiversity of beech and black pine stands in the Balkans
- Prof. Nives Ogrinc 14. Groundwater age determination in deep aquifers of Slovenia Asst. Prof. Sonja Lojen
- Sediments in aquatic environments: their geochemical and mineralogical characterization, remediation, and use as secondary raw materials Prof. Radmila Milačić
- Petrology of brown (low-rank) coals as mined and/or used in Slovenia, natural gasses in them, and their gas-sorption properties Dr. Tjaša Kanduč
- Dr. pasa Randue
 Carbon dynamics in forest soils and the rhizosphere Prof. Nives Ogrinc
- Optimisation of a polychlorinated biphenyls' (PCBs) contaminated material dump site remediation Prof. Milena Horvat
- Vulnerability assessment and identification of suitable remediation measures in degraded ecosystem – a case study of the Idrija mercury mine region Dr. David Koeman
- Psychoactive pharmaceuticals and their transformation products in water treatment processes
- Dr. Tina Kosjek
- 21. Farming possibilities in water protection areas Asst. Prof. Sonja Lojen
- 22. Efficiency of SÉA and health impact assessment in strategic evaluation of plans Prof. Branko Kontić
- The use of specific methods for determination and prevention of adulteration of milk and dairy products Prof. Nives Ogrinc
- 24. Quality of fish on Slovenian market and analysis of possibilities to adjust supply to demand with respect to secure nutritional safety and increase competitiveness of fisheries and aquaculture(Healthy fish - healthy as fisH Prof. Vekoslava Stibilj
- Monitoring of some pollutants in foodstuffs Asst. Prof. Zdenka Šlejkovec
- 26. Expert opinion, attendance at the expert meeting and presentations for the aspects of major accident prevention and Mercury pollution in the Gulf of Trieste Prof. Milena Horvat
- 27. SCOPES; Eradication of lung cancer caused by radon gas in Azerbaijan and Slovenia Prof. Janja Vaupotič

NEW CONTRACTS

- Off-site radiological monitoring of NPP Krško 2011-2013 Krško Nuclear Power Plant Prof. Vekoslava Stibili
- Consultancy on environmental impact evaluations related to planned NPP2 Krško Gen, d. o. o.
- Prof. Branko Kontić
- Ecology laboratory with mobile unit Ministry of Defence
- Dr. Dušan Žigon 4. Co-financing of activities of holder of national standard in 2012 - amount of substance / soil

Ministry of Economic Development and Technology Dr. Polona Vreča

- Ilona Matveyeva, Al-Farabi Kazakh National University, Almaty, Kazakhstan, 15. 2.–14.
 2012 and 24. 9.–21. 12. 2012
- Dr. Borbála Máté, Institute of Radiochemistry and Radioecology, University of Pannonia, Veszprém, Hungary, 13. 3.–12 4. 2012
- Dr. Alexey Ekaykin, Arctic and Antarctic Research Institute, St. Petersburg, Russian Federation, 16-19.4. 2012
- 9. Iva Todoranova, State Enterprise for Radioactive Waste, Sofia, Bulgaria, 16–27. 4. 2012 and 3–7. 9. 2012



- Rositza Kamenova-Totzeva, National Centre of Radiobiology and Radiation Protection, Sofia, Bulgaria, 16–27. 4. 2012
- Oana Dumitru Rusu, Babes-Bolyai University, Cluj-Napoca, Romania, 16–27. 4. 2012 and 3–7. 9. 2012
 Dr Elke Bozau TU Clausthal Clausthal-Zellerfeld Germany 16. 4 –11. 5. 2012 and
- Dr. Elke Bozau, TU Clausthal, Clausthal-Zellerfeld, Germany, 16. 4.–11 5. 2012 and 26. 8.–2. 9. 2012
- Mária Horváth, Institute of Radiochemistry and Radioecology, University of Pannonia, Veszprém, Hungary, 24. 4.–12. 5. 2012
- Dr. Tibor Kovács, Institute of Radiochemistry and Radioecology, Pannonian University, Veszprém, Hungary, 11–12. 5. 2012
- Jelena Lušić, Institute of Oceanography and Fisheries, Split, Croatia, 14. 5.–8. 6. 2012
 Dr. Neven Cukrov, Dr. Ivanka Pižeta, Dr. Ivanka Lovrenčić Mikelić, Dr. Dario Omanović, Ruđer Bošković Institute, Zagreb, Croatia 16. 5. 2012
- 17. Dr. Dario Omanović, Ruđer Bošković Institute, Zagreb, Croatia, 3-7. 6. 2012
- Dr. Ludovit Mifkovič, Dr. Miroslav Jeskovsky, Dr. Maria Šivova, Dr. Pavel Povinec, Comenius University in Bratislava, Bratislava, Slovakia, 25.6.-7. 7. 2012
- Lukasz Plesniak, University of Wrocław, Wrocław, Poland, 3. 5.–29. 6. 2012
 Dr. Akagi Hirokatsu, Dr. Akagi Junko, Prof. Imura Ryusuke, Dr. Kodamatani Hitoshi, Dr. Matsuyama Akito, Dr. Tomiyasu Takashi, National Institute For Minamata Disease, Kumamoto, Japan, 28. 5.–1. 6. 2012
- Yuliya Marchuk, Aykerym Kozhamberdina, Al-Farabi Kazakh National University, Almaty, Kazakhstan, 3–20. 6. 2012
- Andreea Teodor, Ministry of Health, National Institute of Public Health, Iasi, Romania, 11–22. 6. 2012
- 23. Elida Bylyku, Centre of Applied Nuclear Physics, Tirana, Albania, 11-22. 6. 2012
- 24. Georgi Slavchev Georgiev, State Enterprise Radioactive Waste, Bulgaria, 11-22. 6. 2012
- Jordanka Anuseva, Institute of Public Health of Republic of Macedonia, Skopje, Macedonia, 11–22. 6. 2012
- 26. Yan Lin, Norwegian Institute for Water Research, Oslo, Norway, 11-30. 6. 2012
- Dr. Neven Cukrov, Dr. Ivanka Pižeta, Dr. Ivanka Lovrenčić Mikelić, Ruđer Bošković Institute, Zagreb, Croatia, 4. 7. 2012
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- 13. Prof. Nives Ogrinc
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- 16. Prof. Janez Ščančar
- 17. Asst. Prof. Zdenka Šlejkovec
- 18. Prof. Janja Vaupotič
- 19. Dr. Polona Vreča

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21. Dr. Urška Dermol

- 22. Dr. Tjaša Kanduč
- 23. Dr. Davor Kontić
- 24. Dr. Darja Mazej
- 25. Dr. Andrej Osterc, left 01.09.12
- 26. Dr. Marko Štrok
- 27. Dr. Mitja Vahčič
- 28. Dr. Tea Zuliani

Postgraduates

29. Dr. Miha Avberšek, left 02.07.12

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- Dr. Oleksandr Lyashchuk, National Antarctic Scientific Centre of the State Agency on Science, Innovations and Informatization of Ukraine, Kiev, Ukraine, 2. 9.–10. 10. 2012
- 30. Sultan Uzun, Turkey Atomic Energy Authority (TAEK), Istanbul, Turkey, 3-7. 9. 2012
- 31. Dr Elida Bylyku, Centre of Applied Nuclear Physics, Tirana, Albania, 3-7. 9. 2012
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 Prof. Tatiana Zelentsova, Prof. Vitaliy Rusov, Dr. Vladimir Smolyar, Department of Theoretical and Experimental Nuclear Physics, Odessa National Polytechnic University, Odessa, Ukraine, 10. 9.–10. 10. 2012
- Christiana Odumah Anderson, Department of Physics, University of Cape Coast, Cape Coast, Ghana, 1. 10.–24. 12. 2012
- 36. Dr. Ivanka Mikelić, Ruđer Bošković Institute, Zagreb, Croatia, 7–12. 10. 2012
- 37. Dr. Bojan Hamer, Emina Durmiši, Ruđer Bošković Institute, Zagreb, Croatia, 12. 10. 2012
- 38. Mihriban Şengör, Turkish Atomic Energy Authority (TAEK), Ankara, Turkey, 15-26. 10 2012
- 39. Aylin Kurt, Turkish Atomic Energy Authority (TAEK), Ankara, Turkey, 15-26. 10 2012
- Prof. Gaye Çakal, Rufiyet Kurt, Ankara University, Institute of Nuclear Sciences, Ankara, Turkey, 15–26. 10 2012
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- 42. Mihaela Silvia Stoica, Institute for Nuclear Research, Pitesti, Romania, 15-26. 10 2012
- Dr. Danijela Ašperger, Dr. Sandra Babić, Dr. Dragana Mutavdžić Pavlović, Martina Periša, Mirta Zrnčić, Faculty of Chemical Engineering and Technology, Zagreb, Croatia, 29. 11.–1. 12. 2012
- Dr. Stephan Boesereilly, Dr. Nadie Steckling, Sonja Ramlow, Bielefeld University, School of Public Health, University for Health Sciences, 17. 12. 2012
- Dr. Maria Ângela de Barros Correia Menezes, CDTN/CNEN (Nuclear Technology Development Center/Brazilian Commission for Nuclear Energy), Belo Horizonte, Minas Gerais, Brazil, 3–24. 6. 2012 and 11–25. 11. 2012
- Dr. Zora S. Žunić, Dr. Predrag Kolarž, Vinča Institute of Nuclear Sciences, Belgrade in Institute of Physics, Belgrade, Serbia, 17–23. 12. 2012
- 30. Ermira Begu, B. Sc.
- 31. Mateja Bezek, B. Sc.
- 32. Arne Bratkič, B. Sc.
- 33. Marko Černe, B. Sc.
- 34. Marjeta Česen, B. Sc
- 35. Marinka Gams Petrišič, B. Sc.
- 36. Asta Gregorič, B. Sc.
- 37. Urška Kristan, B. Sc.
- 38. Anže Martinčič, B. Sc.
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- 40. Petra Novak, B. Sc.
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- 42. Tina Oblak, B. Sc.
- 43. Majda Pavlin, B. Sc.
- 44. Kelly Peeters, B. Sc.
- 45. Kristina Pestotnik**
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- 47. Janja Snoj Tratnik, B. Sc.
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- 49. Saša Zavadlav, B. Sc.
- 50. Dr. Andreja Zelenik Pevec, left 01.06.12
- 51. Mojca Zupanc**

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- 52. Vesna Fajon
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- 55. Janja Smrke
- 56. Barbara Svetek, B. Sc.
- 57. Zdenka Trkov, B. Sc.
- 58. Stojan Žigon
- ** postgraduate financed by industry

BIBLIOGRAPHY

ORIGINAL SCIENTIFIC ARTICLE

- 1. Alessandro Acquavita, Stefano Covelli, Andrea Emili, Daniela Berto, Jadran Faganeli, Michele Giani, Milena Horvat, Neža Koron, Federico Rampazzo, "Mercury in the sediments of the Marano and Grado Lagoon (northern Adriatic Sea): sources, distribution and speciation", *Estuar., coast. shelf sci.*, vol. 113, pp. 20-31, 2012.
- 2. Franco Baldi, Michele Gallo, Davide Marchetto, Renato Fani, Isabel Maida, Milena Horvat, Vesna Fajon, Suzana Žižek, Mark E. Hines, "Seasonal mercury transformation and surficial sediment detoxification by bacteria of Marano and Grado lagoons", *Estuar., coast. shelf sci.*, vol. 113, issue 10, pp. 105-115, 2012.
- Franco Baldi, Davide Marchetto, Michele Gallo, Renato Fani, Isabel Maida, Stefano Covelli, Vesna Fajon, Suzana Žižek, Mark E. Hines, Milena Horvat, "Chlor-alkali plant contamination of Aussa River sediments induced a large Hg-resistant bacterial community", *Estuar., coast. shelf sci.*, vol. 113, issue 10, pp. 96-104, 2012.
- 4. Karmen Bat, Rajko Vidrih, Marijan Nečemer, Branka Mozetič Vodopivec, Ines Mulič, Peter Kump, Nives Ogrinc, "Characterization of Slovenian apples with respect to their botanical and geographical origin and agricultural production practice", *Food technol. biotechnol.*, vol. 50, no. 1, pp. 107-116, 2012.
- Ljudmila Benedik, Zvonka Jeran, "Radiological of natural and mineral drinking waters in Slovenia", *Radiat. prot. dosim.*, no. 2, vol. 151, pp. 306-313, 2012.
- 6. Mateja Bezek, Asta Gregorič, Norbert Kávási, Janja Vaupotič, "Diurnal and seasonal variations of concentration and size distribution of nanoaerosols (10-1100 nm) enclosing radon decay products in the Postojna Cave, Slovenia", In: Proceedings of the NARE 2012, International Symposium on Natural Radiation Exposures and Low Dose Radiation Epidemiological Studies, 1-3 March 2012, Hirosaki, Japan, *Radiation protection dosimetry*, vol. 152, no. 1/3, pp. 174-178, 2012.
- Mateja Bezek, Janja Vaupotič, "Nanoaerosols including radon decay products in outdoor and indoor air at a suburban site", *J. Toxicol.*, vol. 2012, pp. 510876-1-510876-31, 2012.
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- 9. Arne Bratkič, Martina Burnik Šturm, Jadran Faganeli, Nives Ogrinc, "Semi-annual carbon and nitrogen isotope variations in the water column of Lake Bled, NW Slovenia", *Biogeosciences (Print)*, vol. 9, no. 1, pp. 1-11, 2012.
- 10. Martina Burnik Šturm, Polona Vreča, Ines Krajcar Bronić, "Carbon isotopic composition (δ^{13} C and ¹⁴C activity) of plant samples in the vicinity of the Slovene nuclear power plant", *J. environ. radioact.*, vol. 110, no. 1, pp. 24-29, 2012.
- 11. Ivana Capan, V. Janicki, Radojko Jaćimović, Branko Pivac, "C-V and DLTS studies of radiation induced Si-SiO₂ interface defects", In: Proceedings of the Ion Beam Synthesis and Modification of Nanostructured Materials and Surfaces, 9-13 May, 2011, Strasbourg, France, Nuclear instruments & methods in physics research, Section B, Beam interactions with materials and atoms, vol. 282, pp. 59-62, 2012.
- 12. Neven Cukrov, Nataša Tepić, Dario Omanović, Sonja Lojen, Elvira Bura-Nakić, Vjeročka Vojvodić, Ivanka Pižeta, "Qualitative interpretation of physico-chemical and isotopic parameters in the Krka River (Croatia) assessed by multivariate statistical analysis", *Int. j. environ. anal. chem.*, vol. 92, issue 10, pp. 1187-1199, 2012.
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- 14. Erica Donner, Tina Kosjek, Signe Qualmann, Kresten Ole Kusk, Ester Heath, D. Michael Revitt, Anna Ledin, Henrik Rasmus Andersen, "Ecotoxicity of carbamazepine and its UV photolysis transformation products", *Sci. total environ.*, vol. 443, pp. 870-876, 2012.
- 15. Stevo Dozet, Tjaša Kanduč, Miloš Markič, "A contribution to petrology of dark grey to black interbeds within Upper Permian and Triassic

carbonate rocks in the area between Ljubljana and Bloke, Central Slovenia", *Geologija*, vol. 55, no. 1, pp. 77-92, 2012.

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DEPARTMENT OF AUTOMATION, **BIOCYBERNETICS AND ROBOTICS** E-1

The research strategy within our department is unique, as it supports a variety of multi- and interdisciplinary research projects. Specifically, our research combines the fields of automatics, robotics (including intelligent control, humanoids, cognitive robotics, and robot vision), biocybernetics, kinesiology, ergonomics and environmental physiology. The common theme in all our research endeavours has been optimising the "behaviour of man and machine", accounting for interactions with the environment. In the past year we have added "human-robot partnership" as an additional goal of our research programme. By combining engineering sciences and life sciences we have been able to make significant contributions to the development of the following: new methods for sensorimotor learning by imitation and coaching, a planetary habitat simulation facility, humanoid vision systems, manikins enabling the evaluation of protective garments for industry and recreation, kinematic models of the human body that serve as a basis for the design of anthropomorphic systems, and a medical treatment for frostbite.



The department maintains the Programme Group "Automatics, robotics and biocybernetics" in Head: the field of Production Technology. This Programme Group has three major overlapping research Asst. Prof. Leon Žlajpah foci: automation and intelligent control (leader: doc. dr. Leon Žlajpah), humanoid and cognitive robotics (leader: dr. Aleš Ude), and biocybernetics: environmental physiology & ergonomics (leader: prof. dr. Igor B. Mekjavic). By maintaining a critical mass of researchers in all three areas within one Programme Group we have managed to foster exciting multidisciplinary projects.

During 2012 the main research topics in the department included humanoid robotics, the control of robot systems and learning strategies, studies of human physiology in extreme environments, the evaluation of protective equipment, the development of biomedical methods, and the automation of industrial manufacturing.

Automation and Intelligent Control

The research orientation within this group is primarily in the development of advanced control strategies for robot systems working in unstructured environments, low-level reflexive control, bio-inspired control systems, cooperating robot systems and the automation of industrial processes.

Note: Since its inception the department has maintained an inter- and multidisciplinary research focus. The founders provided a scientific inheritance that includes pioneering research culminating in the first demonstration of how functional electrical stimulation can help paraplegics to walk, and the development of the first industrial robots in our region. In addition to kinematics, the common denominator in biomedical and robotic research is improving the quality of life.

Advanced robot control

We developed a method for the control of kinematically redundant robots, where we focus on a smooth, continuous transition between the primary and the secondary tasks. The proposed method is general. It was demonstrated by simulation and on real robots for ensuring the reflex stability of humanoid robots and as well as for obstacle-

avoidance tasks. The method was implemented on a skiing robot, on the humanoid robot HOAP-3 and on the humanoid robot CB-I in cooperation with Advanced Telecommunications Research Institute International (ATR).

We analysed the properties of a biped version of the spring-loaded inverted pendulum (biSLIP), which in some cases shows open-loop stable behaviour. The sets of parameters (initial energy, spring constant, attack angle, etc.) which led to the open-loop stable behaviour were determined based on the simulations. For the generation of humanoid walking cycles we proposed a novel control architecture, which includes movement prototypes or motor primitives with the corresponding task/joint dynamics implemented as an extended version of dynamical systems (DMPs). The method was tested and evaluated in simulations.



Figure 1: Transfer of interactive force skills through augmented reality tele-operation

Robot-motion synthesis through human sensorimotor learning

We extended our novel paradigm where a human can teach a robot new skills by exploiting human sensorimotor ability, to dynamical full-body skills. To provide the human with a feedback that is suitable for full-body robot

We have designed a novel machine-learning scheme that enables a robot to learn the task simultaneously while the human is operating the robot, and that gradually transfers the control responsibility from the human to the incrementally built autonomous robot controller. s. To provide the human with a feedback that is suitable for full-body robot control we constructed a haptic interface that stimulates the human senses by influencing the human centre-of-mass. The motion of the centre-of-mass is one of the key pieces of information for the dynamic control of the human body. This interface reproduced the force to the human centre-of-mass, which provided the feedback for robot dynamics. To evaluate the feasibility of this approach and the proposed type of feedback we conducted two full-body experiments. In the first experiment, a human had to teach the robot how to compliantly interact with another human. In this experiment the human

held robot hands and arbitrarily pushed and pulled them. The robot sensory system detected the interaction and the human demonstrator had to react on the given feedback to follow the intention of the interaction. Besides moving the hands into the direction of the applied force, the robot centre-of-mass also had to be kept in a stable position. The results of the experiment showed that the human was able to teach the robot about the described interaction. In the second experiment the task was to teach a humanoid robot how to maintain the postural stability in the presence of the perturbations. Here we designed a novel machine-learning scheme that enabled the robot to learn the task simultaneously, while the human is operating the robot. Basically, we combined the Locally Weighted Projection Regression machine-learning method with a novel approach to gradually transfer the control responsibility from the human to the incrementally built autonomous robot controller.

Exoskeletons for augmenting human-motion ability

A recent trend in robotics is to design special exoskeleton mechanisms to either augment the abilities of ablebodied humans or to substitute/improve the condition of people with impaired physical abilities. A number of studies discuss the design and control of such mechanisms, yet relatively few address the effect on the energy expenditure of the user. In this research we studied the effect of a performance-augmenting exoskeleton on the metabolic cost of an able-bodied user during periodic squatting. We investigated whether an exoskeleton device reduces the metabolic cost and what is the influence of the chosen device control strategy. By measuring the oxygen consumption, minute ventilation, heart rate, blood oxygenation and muscle EMG during a 5-minute squatting series, we showed the effects of using a prototype robotic knee exoskeleton under three different non-invasive control approaches:



Figure 2: Integrating visual perception and manipulation for the learning of new object representations (in collaboration with ATR Computational Neuroscience Laboratories, Kyoto, Japan)

a gravity-compensation approach, a position-based approach and a novel oscillator-based approach. The latter proposes a novel control that ensures synchronization of the device and the user. A statistically significant decrease in physiological responses can be observed when using the robotic knee exoskeleton under gravity compensation and oscillator-based control. On the other hand, the effects of position-based control were not significant in all parameters, although all the approaches significantly reduced the energy expenditure during squatting.

ICT in sport

We developed special force plates for measuring the forces in alpine skiing based on TexScan force load cells. The force plate consists of a bottom, which is attached to the skis and enables free flex motion, and an upper part, which contains load cells and vertical guides. We have tested the developed equipment in the laboratory as well as on the ski slope. Unfortunately, it has turned out that the TexScan sensors are not suitable for outdoor measurements. Therefore, we developed new force plates using strain gauges based sensors. In order to avoid a cable connection between the force plates and the data logger, we developed a wireless communication using Bluetooth protocol.

Design of robot mechanisms

Experimental work with two-arm robots has shown that for motion planning for humanoid robots it is also necessary to imitate the motion of the human spine, especially the motion of the spinal arc. Therefore, we have developed a prototype of a torso for a humanoid robot on which the robot arms will be mounted. We designed different solutions and by using 3D simulations we selected two of them, which perform the movement very similar to the human spine. In both versions there are three parallel bar mechanisms set in series, one above the other. In this

way the proposed mechanism achieves a perfect imitation of the motion of the spinal arc. The difference between the solutions is in the transfer of the torques to the next higher lying segment. While the first mechanism is using a direct transfer rod, the other uses gears for the torque transmission. For the mechanism with the transfer rod we made a prototype. Since the design solution is original and new, we submitted a patent application.

Automation, robotics and factory information systems for manufacturing

In 2012 we continued our cooperation with a glass company that develops and produces a large range of glassware with a novel R&D project "The development of an automated glass blowing cell". Our target is to automate glassblowing, the most important operation in several company production cells for various type of ceiling lights

and other lamp types. The present specific manual glass blowing is the most demanding operation that only a couple of skilled workers perform satisfactorily. To identify the important process characteristics, we have done a number of targeted measurements and experiments. Then, we designed the overall structure of a system for automatic glassblowing. We conceived a method for the formal representation of automated glassblowing and the method for its construction. These are determined by performing particular measurements of manual glassblowing for each item, specific data processing and the representation of extracted data in a form that encompass all the relevant information. We developed all the hardware components of the automated cell, like computer control, special electro-pneumatic devices and sensor subsystems. We conceived the various methods needed for automated control and implemented them in the controller program system. The devel- Figure 3: Discovering new motor primitives through graph search oped system consists of industrially robust subsystems that are integrated



into the existing production environment. The automated glassblowing system has been deployed and tested in the actual production and a number of improvements have been made. At the start of 2013 we will carry out measurements on all the items in the product range and construct the related representations for automated glassblowing.

Humanoid and Cognitive Robotics Lab

The aim of the research within the area of humanoid and cognitive robotics is to create robots capable of helping people and interacting with them in natural environments. Since humanoids are similar to humans, it is much easier for people to interact with humanoids than with other types of robots. As a result we believe that cognitive humanoid robots are the key to the development of robot companions that can help people in their homes, which is one of the most important challenges for robotics research.

The Humanoid and Cognitive Robotics lab is involved in a number of EU projects from the program "Cognitive Systems and Robotics". Most of our work in 2012 was performed within two FP7 projects, Xperience and IntellAct:

large-scale integrated project "Robots bootstrapped through learning from experience" (Xperience), which has 7 partners.

STREP project "Intelligent observation and execution of actions and manipulations" (ItellAct) with 6 partners. A more detailed description of both projects follows below.

Xperience (http://www.xperience.org/)

Current artificial cognitive systems are limited with respect to the generative mechanisms that rely on prior knowledge are employed to predict the immediate future and are the key to increasing the bandwidth and speed of cognitive development. The goal of Xperience is to demonstrate that state-of-the-art enactive systems can be significantly extended by using structural bootstrapping to generate new knowledge. This process is founded on explorative knowledge acquisition, and subsequently validated through experience-based generalization. In Xperience we are going to implement, adapt, and extend a complete robot system for automating the introspective, predictive, and interactive understanding of actions and dynamic situations.

IntellAct (http://intellact.eu/)

In this project we address the problem of understanding and exploiting the meaning (semantics) of manipulations in terms of objects, actions and their consequences for reproducing human actions with machines. This is

in particular required for the interaction between humans and robots, in which the robot has to understand the human action and then transfer it to its own embodiment. IntellAct aims to provide the means to allow for this transfer, not by copying the movements of the human but by transferring the human action on a semantic level. IntellAct will demonstrate the ability

We developed a new robot-learning concept that combines robot programming by demonstration and reinforcement learning.

to understand scene and action semantics and to execute actions with a robot in two domains. Firstly, in a laboratory environment (exemplified by a lab on the International Space Station (ISS)), and secondly, in an assembly process in an industrial context.

Our most important result in 2012 was the development of a new robot learning concept that combines robot programming by demonstration and reinforcement learning. Robot programming by demonstration (RPD) is an important idea that helps us limit the search space when programing high-degree-of-freedom robotic systems like humanoid robots. However, RPD requires the acquisition of many example movements that solve the desired task in different situations. The example movements are acquired with the help of a human teacher. To reduce the workload on the human teacher and enable a more autonomous form of learning, we integrated robot programming by demonstration and reinforcement learning; RPD is used to acquire a small number of initial examples that provide the scaffolding for reinforcement learning. On the other hand, reinforcement learning provides new examples that are suitable for inclusion in the action library. We demonstrated how this concept can be applied to quickly solve a number of difficult robot control learning problems.

ACAT

In 2012 (Call 9 of the EU program Cognitive Systems and Robotics) we acquired a new project with the title Learning and Execution of Action Categories (ACAT). This project focuses on the problem of how artificial systems (robots) can understand and utilize information made for humans. For this, ACAT generates a dynamic process



Figure 4: Integration of the automated solution in the production environment.

memory by the extraction and storage of action categories from large bodies of human-compatible sources (text, images). The action categories are designed to include the actual action-encoding but also large amounts of context information ("background"). The ACAT system then uses actioncategories to compile robot-executable plans. The execution benefits strongly from the rich context information present in the action-categories, which allows for generalization (for example, replacement of objects in an action). It also permits us to specifically address ambiguity, incompleteness and uncertainty in planning. The plans are grounded by perception and execution, which takes place by a robot. This leads to a life-long update process of the knowledge base.

The ultimate purpose of ACAT is to equip the robot – on an on-going basis – with abstract, functional knowledge, normally made for humans, about relations between actions and objects leading to a system that can act meaningfully. As an industrially relevant scenario, ACAT uses "instruction sheets" (manuals), made for human workers, and translates these

into a robot-executable format. In this way the robot will be able to partially take over human tasks without timeconsuming programming procedures. Similar to computer science, where the development of the first compilers led to a major step forward, the main impact of this project is that ACAT develops a robot-compiler, which translates human-understandable information into a robot-executable program.

Research in the area of humanoid and cognitive robotics is further conducted within a number of smaller projects supported by the Slovenian Research Agency and other international entities, as well as with funding

A new FP7 specific targeted research project (STREP) was acquired within the EU Framework Programme 7 "Cognitive Systems and Robotics: "Learning and Execution of Action Categories". Research Agency and other international entities, as well as with funding acquired in the frame of the young researchers' program. All these projects focus on a better understanding of sensorimotor learning, visual processing, and lifelong learning in robotic systems, thus contributing to the overall vision of the group. We have published our results in prime robotics journals, including IEEE Transactions on Robotics.

Biocybernetics (Environmental Physiology & Ergonomics)

Research within our Biocybernetics Group focuses primarily on projects concerning the influence of extreme environments on humans, and the development and evaluation of technology and strategies to maintain safety and unhindered performance in such environments.

Planetary Habitat Simulation

The aim of this research programme is to investigate the effect of planetary habitat environments on human physiological systems. For technical reasons, the environment within future Lunar and Mars habitats will be hypobaric. Despite the elevated levels of oxygen in these habitats, astronauts will be exposed to hypobaric hypoxia. Prolonged exposure to low gravity results in a deconditioning of vital physiological systems, and may consequently constitute a threat to the health of the astronauts. However, it is unknown how prolonged exposure to both reduced gravity and hypoxia will affect health. For the purpose of this research programme we established a Planetary Habitat Simulation Facility at the Olympic Sport Centre Planica. The challenge of the project is in the complexity of the experimental interventions, whereby healthy humans are confined to a hypoxic environment during prolonged bedrest. Subjects have recently participated in three trials: hypoxic bedrest (simulated altitude 4000m), normoxicbedrest, and hypoxic ambulation. The effects of these interventions were investigated in experiments concerning metabolic, cardiorespiratory, musculoskeletal, haematological, immunological and thermoregulatory functions. We anticipate that the new knowledge gleaned

A series of studies funded by the European Space Agency (ESA) Programme for European Cooperating States (PECS) have been completed at the Planica hypoxia facility. A new research programme has now been established, funded by the EU Framework programme (FP7), which addresses the effects of longer exposure to combined inactivity/unloading and hypoxia.

from these studies will have implications for society in general, since chronic hypoxia and bedrest constitute a model of the basic conditions experienced by patients suffering from respiratory insufficiency, thereby restricting them to a physically inactive life style.

Hypoxia and weight loss

The mechanism of weight loss observed during prolonged sojourns at high altitude does not appear to be entirely due to an imbalance between energy intake and expenditure. The observation that high-altitude exposure may lead to considerable weight loss has led to the suggestion that it might be beneficial to incorporate hypoxic training in weight management programmes for obese individuals. Studies have demonstrated that mild physical exercise in normobaric hypoxia causes a significantly greater weight loss in obese persons than exercise in a sham hypoxic environment. To the best of our knowledge, no systematic studies have been carried out to date regarding the treatment of obesity under hypoxic conditions. During prolonged sojourns to high altitude, factors which may contribute to weight loss include: dehydration, primary anorexia, lack of palatable food, detraining, and possibly direct effects of hypoxia on metabolism. We have completed a series of studies, co-financed by a Dutch industrial partner b-Cat, investigating the effect of 10-d sojourns in normobaric hypoxia, equivalent to a simulated altitude of 3200 m, on the metabolism. Specifically, the responses of plasma glucose, insulin, gut peptides, resting energy expenditure and satiety scores following a standard meal. Preliminary results indicate that one of the main contributors implicated in the observed weight loss is the elevated resting energy expenditure, and reduced appetite. We have continued this research programme, and are now investigating how different levels of activity influence this hypoxia-induced loss of body mass.



Figure 5: The Planica Facility (Olympic Sport Centre Planica), built with EU Regional Development Funds, is the site of our Planetary Habitat Simulations. Our department collaborated with the industrial partner b-Cat in designing and installing the Vacuum Pressure Swing Adsorption (VPSA) system, capable of maintaining hypoxia in one entire floor (in the building on the left) at levels equivalent to altitudes up to 5400 m. Medical research studies were conducted to assess the combined effects of hypoxia and inactivity on physiological systems.

Sleep architecture during exposure to hypoxia

With colleagues from the Institute of Neurophysiology at University Clinical Centre Ljubljana we are investigating the effect of sleep architecture during prolonged exposure to hypoxia combined with different levels of activity. Our findings to date indicate that although there is no effect of sleep architecture, the main effect is on the frequency and magnitude of sleep apnea.

Sleep temperature regulation

In addition to the polysomnographic recordings, we have also tested the theory that sleep onset is functionally linked with thermoafferent feedback from cutaneous warm receptors. Our preliminary results confirm this theory, but have revealed that the hypoxia-induced vasoconstriction observed during the day disappears during the night. Our current research has focussed on gaining a better understanding of this phenomenon.

Altitude retinopathy

Using a non-mydriatic fundus camera we have documented the diameter of retinal arterioles and venules at different stages of hypoxic exposure. Together with colleagues from the Eye Clinic at the University Clinical Centre, and the VITO Institute in Belgium, we are currently analysing these scans to assess any hypoxia-induced vascular changes in the retina, which may be related to the onset of altitude retinopathy.

Broadpeak and MuztaghAta

In addition to our laboratory investigations we continue to collaborate with high-altitude Slovene expeditions, assisting with their preparations and monitoring the effects of the high-altitude exposures on various physiological systems. In 2012 we provided research support for two expeditions, one to Broadpeak, and the other to Muztagh Ata.

Development of a diagnostic tool for determining susceptibility to freezing cold injury

In Slovenia the main risk group for cold injury are alpinists participating in high-altitude expeditions. In collaboration with researchers from the Royal Institute of Technology (Stockholm, Sweden), we have initiated a research program that has two specific aims: i) to develop a diagnostic method to determine the susceptibility of



Figure 6: Using infrared thermography to monitor hand and foot digits following immersion in cold water, we have been able to classify individuals into high- and low-risk groups for cold injury.

c aims: i) to develop a diagnostic method to determine the susceptibility of individuals to cold injury; ii) to develop a training program to improve an individual's vascular response to a cold stimulus, thus minimizing one's risk to cold injury. A series of laboratory and field studies have been conducted examining the digit vascular response to cold-water immersion (cold-induced vasodilatation, CIVD), and the pattern of digit reperfusion following cold exposure using infrared thermography. We are currently evaluating the effect of several training programmes, in terms of their effect on the CIVD response.

Evaluation of protective clothing (Desert Ensembles)

Soldiers on peacekeeping missions in desert regions must be able to sustain prolonged exposures to hot (45°C) and dry (10% relative humidity) environments, all whilst dressed in full combat gear. Our research programme initially focussed on the physiological responses of soldiers carrying loads in such environments. We have continued our work in this area, and have evaluated the efficacy of different technologies (i.e., ventilated vests) and/or strategies (i.e., work/rest schedules) in minimising heat strain and improving the performance in such environments. Together with colleagues from the Royal Institute of Technology we have continued this work to assess the impact of the next-to-skin layer on the thermal balance of soldiers in such environments. In addition, we have also investigated the

effect of moisture content of the next-to-skin layer on a predicted burn injury during a simulated flash fire. With the industrial partner Lenzing (Austria) we have demonstrated that increased moisture content of the next-to-skin layer provides added protection against burn injury. We are continuing our analysis to determine under what conditions the microenvironment moisture may lead to scalding injury.

Some outstanding publications in the past three years

- 1. Petrič, T., Gams, A., Ijspeert, A. J., Žlajpah, L.: On-line frequency adaptation and movement imitation for rhythmic robotic tasks, Int. j. rob. res., 2011, vol. 30, no. 14, pp. 1775–1788
- 2. Ude, A., Gams, A., Asfour, T., Morimoto, J.: Task-specific generalization of discrete and periodic dynamic movement primitives. IEEE trans. Robot. [Print ed.], 2010, vol. 26, no. 5, pp. 800–815
- Nemec, B., Ude, A.: Action sequencing using dynamic movement primitives, Robotica, 2012, vol. 30, no. 5, pp. 837–846
- Babič, J., Hale, J. G., Oztop, E.: Human sensorimotor learning for humanoid robot skill synthesis, Adapt. behav., 2011, vol. 19, no. 4, pp. 250–263
- 5. Mekjavić, I. B., Dobnikar, U., Kounalakis, S. N.: Cold-induced vasodilation response in the fingers at four different water temperatures. Applied physiology, nutrition and metabolism, 2013, [in press]
- 6. Kounalakis, S. N., Eiken, O., Mekjavić, I. B.: Exercise thermoregulatory responses following a 28-day sleep-high train-low regimen. Eur. j. appl. physiol., 2012, [Print ed.]
- Debevec, T., Mekjavić, I. B.: Short intermittent hypoxic exposures augment ventilation but do not alter regional cerebral and muscle oxygenation during hypoxic exercise. Respiratory physiology & neurobiology, 2012, vol. 181, no.2, pp. 132–142

Awards and appointments

- 1. Dr. Jan Babič, Luka Peternel: Best Paper Student Award at a conference Robotics in Alpe-Adria-Danube Region 2012, Naples, Italy (awarded by the conference organizers)
- Dr. Andrej Gams received the Jožef Stefan Golden Emblem for his Ph.D. He was nominated for the award by prof. Tadej Bajd from the Faculty of Electrical Engineering, University of Ljubljana. The award is presented by the Jožef Stefan Institute
- 3. Dr. Shawnda Morrison: Research Trainee Fellowship, Michael Smith Foundation for Health Research Fellowship, University of British Columbia, Kelowna, BC, Canada
- 4. Dr. Aleš Ude: Award for the paper titled "Integrating surface-based hypotheses and manipulation for autonomous segmentation and learning of object representations", which was the finalist for the best-cognitive-paper award at the IEEE International Conference on Robotics and Automation (ICRA), held in St. Paul, MN, USA. ICRA is a prime conference in the area of robotics worldwide

Annual Report 2012

INTERNATIONAL PROJECTS

- Co-financing of the hypoxic and hyperoxic exercise B-Cat B. V. Prof. Igor Mekjavić
- 7. FP IntellAct: Intelligent observation and execution of actions and manipulation European Commission Asst. Prof. Aleš Ude
- 7. FP Xperience: Robots bootstrapped through learning from experience European Commission
- Asst. Prof. Aleš Ude
- 7. FP ICARUS: International cooperation for the advancement of researcher on the undrelaying system of human thermoregulation European Commission
- Prof. Igor Mekjavić 5 7 FP - PlanHah: Planetary babit.
- 7. FP PlanHab: Planetary habitat simulation European Commission Prof. Igor Mekjavić
- ESA: Planetary (Lunar & Mars) habitat simulations PLANICA ESA/ESTEC Prof. Igor Mekjavić
- BI-FR/11-12-PROTEUS-004: Development of an artificail skin as element of sweating thermal manikin Slovenian Research Agency
 - Prof. Igor Mekjavić

RESEARCH PROGRAM

1. Avtomation, robotics and biocybernetics Prof. Igor Mekjavić

R & D GRANTS AND CONTRACTS

1. Dual nature of stem cells in cancer and their application in therapy Prof. Igor Mekjavić

- The role of small GTPases in the regulation of endosomal/lysosomal transport in astrocytes
- Prof. Ígor Mekjavić3. Robot motion synthesis through human visuo-motor learning Asst. Prof. Jan Babič
- 4. Goal directed action synthesis using a library of example movements Asst. Prof. Aleš Ude
- Learning, analysis, and detection of motion in the framework of a hierarchical compositional visual architecture Asst. Prof. Aleš Ude
- The detection of irregularities and fraud in the financing of the public health services Rok Okorn, B. Sc.
- Development of a new generation of thermal manikin for evaluation of personal protective equipment and safety of health in extreme working and living environmental conditions (x-termoman) Prof. Igor Mekjavić
- 8. Influence of ski width on alpine skiing safety
- Asst. Prof. Bojan Nemec
- 9. Hypoxic and hyperoxic exercise
- Prof. Igor Mekjavić 10. Zero and reduced gravity simulation: the effect on the cardiovascular and
- musculoskeletal systems Prof. Igor Mekjavić
- Hypoxic inactivity: Implications for heart failure, respiratory insufficiency and obesity Prof. Igor Mekjavić
- 12. Biologically inspired synthesis of periodic movement for a robotic humanoid leg Dr. Andrej Gams

NEW CONTRACT

 Development of an automatic free-blowing process cell for a glass plant Razvojni Center eNeM Novi Materiali, d. o. o. Dr. Anton Ružić

- VISITORS FROM ABROAD
- 1. Dr. Stylianos Kounalakis, Unversity of Athens, Greece, 2. 2.-8. 3. 2012
- 2. Dr. Erhan Oztop, Ozyegin Universtiy, Ozyegin, Turkey, 7.-11. 3. 2012
- Dr. Judith Buehlmeier, Dr. Joern Rittweger, Dr. Jochen Zange, Deutsches Zentrum f
 ür Luft - und Raumfahrt e.V. (DLR), Köln, Germany, 27.–29. 3. 2012
- Dr. Liz Simpson, David Greenfield Human Physiology Unit, B Floor Medical School, QMC, Nottingham, United Kingdom, 27.–29. 3. 2012
- 6. Dr. Minja Tamosiunate, University of Göttingenu, Germany, 31. 5.-2. 6. 2012
- 7. Dr. Stylianos Kounalakis, Unversity of Athens, Greece, 10.–18. 6. 2012
- 8. Dr. Wolfgang Zitz, g. Kern, g. Risch, g. Glaninger, Magna Steyr, Gradec, Austria, 19. 6. 2012
- Dr. Tomas Kulvicius, Dr. Minja Tamosiunate, University of Göttingenu, Germany, 6.–8.9. 2012
 Dr. Katelyn Marsden, University of British Columbia, Okanagan, Kelowna, Canada, 8. 8.–23. 9. 2012
- 11. Dr. Erhan Oztop, Ozyegin University, Turkey, 8.–11. 11. 2012
- 12. Prof. Vincenzo Parenti Castelli with students, University of Bologna, 18. 12. 2012

STAFF

Researchers

- 1. Asst. Prof. Jan Babič
- 2. Dr. Andrej Gams
- 3. Asst. Prof. Igor Kovač
- 4. Prof. Edvard Kramar*, retired 01.10.12
- 5. Dr. Ladislav Lenart, retired 30.07.12
- 6. Prof. Igor Mekjavić
- 7. Asst. Prof. Bojan Nemec
- 8. Dr. Anton Ružić
- 9. Asst. Prof. Aleš Ude

10. Asst. Prof. Leon Žlajpah, Head

- Postdoctorial associates 11. Dr. Fares Jawad Mohd Abu-Dakka
- 12. Dr. Gregor Cigler*
- 13. Dr. Tadei Debevec

14. Dr. Michail Keramidas, left 01.04.12

- 15. Asst. Prof. Marjeta Kramar Fijavž'
- 16. Dr. Shawnda Morrison

Postgraduates

- 17. Mojca Amon*, M. Sc., left 01.05.12
- 18. Miha Deniša, B. Sc.
- 19. Denis Forte, B. Sc.

- 26. Rok Vuga, B. Sc. **Technical officers** 27. Robert Bevec, B. Sc
- 27. Robert Bevec, B. Sc. 28. Borut Lenart, B. Sc.

Nejc Likar, B. Sc.
 Adam Mc Donnell, B. Sc.

22. Rok Okorn, B. Sc.

24. Tadej Petrič, B. Sc.

23. Luka Peternel, B. Sc.

25. Barry Martin Ridge, B. Sc.

- 29. Bogomir Vrhovec, B. Sc.
- Technical and administrative staff
- 30. Tanja Dragojević, B. Sc.
- 31. Dušan Filipič
- 32. Damjan Fink
 33. Marija Kavčič, B. Sc.
- 35. Marija Kavcić, B 34. Matiaž Kocuvan
- 35. Janez Zalar, retired 01.12.12

Note: * part-time JSI member

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ORIGINAL SCIENTIFIC ARTICLE

- 1. Fares Abu Dakka, Francisco Valero, Vicente Mata, "Evolutionary path planning algorithm for industrial robots", *Adv. robot.*, vol. 26, no. 11/12, pp. 1369-1392, 2012.
- Mojca Amon, Michail E. Keramidas, Stylianos N. Kounalakis, Igor B. Mekjavić, "The effect of a sleep high-train low regimen on the finger cold-induced vasodilation response", *High alt. med. biol.*, vol. 13, no. 1, pp. 32-39, 2012.
- 3. Jan Babič, Goran Škorja, "Analysis of musculoskeletal system responses to perturbations during standing posture", *Elektrotehniški vestnik*, vol. 79, no. 1/2, pp. 7-12, 2012.
- 4. Tadej Debevec, Michail E. Keramidas, Barbara Norman, Thomas Gustafsson, Ola Eiken, Igor B. Mekjavić, "Acute short-term hyperoxia followed by mild hypoxia does not increase EPO production: resolving the "normobaric oxygen paradox"", *Eur. j. appl. physiol. (Print)*, vol. 112, no. 3, 1059-1065, 2012.
- 5. Tadej Debevec, Igor B. Mekjavić, "Short intermittent hypoxic exposures augment ventilation but do not alter regional cerebral and muscle oxygenation during hypoxic exercise", *Respiratory physiology & neurobiology*, vol. 181, no.2, pp. 132-142, 2012.
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- 7. Denis Forte, Andrej Gams, Jun Morimoto, Aleš Ude, "On-line motion synthesis and adaptation using a trajectory database", *Robot. auton. syst.*, vol. 60, no. 10, pp. 1327-1339, 2012.
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- Michail E. Keramidas, Stylianos N. Kounalakis, Ola Eiken, Igor B. Mekjavić, "Carbon monoxide exposure during exercise performance: muscle and cerebral oxygenation", *Acta physiologica*, vol. 204, issue 4, pp. 544-554, 2012.
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- 13. Marjeta Kramar Fijavž, Mitja Lakner, Marjeta Škapin-Rugelj, "An equalarea method for scalar conservation laws", *The Anziam journal*, vol. 53, iss. 2, pp. 156-170, 2012.
- 14. Edvard Kramar, "Some properties of algebraic operators on locally convex spaces", *Acta sci. math. (Szeged)*, vol. 78, no. 1-2, pp. 147-161, 2012.
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- 18. Bojan Nemec, Aleš Ude, "Action sequencing using dynamic movement primitives", *Robotica*, vol. 30, no. 5, pp. 837-846, 2012.
- 19. Agnes Psikuta, Dušan Fiala, Gudrun Laschewski, Gerd Jendritzky, Mark Richards, Krzysztof Błażejczyk, Igor B. Mekjavić, Hannu Rintamäki, Richard de Dear, George Havenith, "Validation of the Fiala multi-node thermophysiological model for UTCI application", *Int. j. biometeorol.*, vol. 56, no. 3, pp. 443-460, 2012.

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PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

1. Shawnda A. Morrison, Bojan Rojc, Andrej Pangrc, Judita Jeran, Ola Eiken, Igor B. Mekjavić, Leja Dolenc-Grošelj, "Respiration during sleep in hypoxia and bedrest", In: *Program in zbornik prispevkov*, Symposium on Sleep Disorders with the 28th Dr. Janez Faganel Memorial Lecture, Ljubljana, 5-6 October 2012, Leja Dolenc-Grošelj, ed., Ljubljana, Section for Clinical Neurophysiology of the Slovenian Medical Association, 2012, pp. 31-32.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- 1. Fares Abu Dakka, Bojan Nemec, Aleš Ude, "Peg-in-hole using dynamic movement primitives", In: *RAAD 2012*, 21th International Workshop on Robotics in Alpe-Adria-Danube Region, 10-13 September 2012, Naples, Italy, [S. l.], ESA, = Edizioni Scientifiche e Artistiche, cop. 2012, pp. 143-149.
- 2. Fares Abu Dakka, Aleš Ude, "Minimum time trajectory planning using genetic algorithms and DMPS presentation for industrial robots", In: *Zbornik 15. mednarodne multikonference Informacijska družba IS 2012, 8.-12. oktober 2012, Ljubljana, Slovenia: zvezek A: volume A,* (Informacijska družba), Marko Bohanec, ed., Matjaž Gams, ed., Dunja Mladenić, ed., Marko Grobelnik, ed., Marjan Heričko, ed., Urban Kordeš, ed., Maja Smrdu, ed., Olga Markič, ed., Zvezdan Pirtošek, ed., Jadran Lenarčič, ed., Leon Žlajpah, ed., Andrej Gams, ed., Vladislav Rajkovič, ed., Znaja Urbančić, ed., Mojca Bernik, ed., Ljubljana, Institut Jožef Stefan, 2012, zv. A, pp. 349-352.
- Jan Babič, Tadej Petrič, Tadej Debevec, Andrej Gams, "Kinematic adaptations during repetitive squatting motions using robotic knee exoskeleton", In: *RAAD 2012*, 21th International Workshop on Robotics in Alpe-Adria-Danube Region, 10-13 September 2012, Naples, Italy, [S. l.], ESA, = Edizioni Scientifiche e Artistiche, cop. 2012, pp. 313-317.
- 4. Robert Bevec, Matej Kristan, "A stereo-video system based trajectory recovery of a moving object", In: *Zbornik 15. mednarodne multikonference Informacijska družba IS 2012, 8.-12. oktober 2012, Ljubljana, Slovenia: zvezek A: volume A,* (Informacijska družba), Marko Bohanec, ed., Matjaž Gams, ed., Dunja Mladenić, ed., Marko Grobelnik, ed., Marjan Heričko, ed., Urban Kordeš, ed., Maja Smrdu, ed., Olga Markič, ed., Zvezdan Pirtošek, ed., Jadran Lenarčič, ed., Leon Žlajpah, ed., Andrej Gams, ed., Vladislav Rajkovič, ed., Tanja Urbančič, ed., Mojca Bernik, ed., Ljubljana, Institut Jožef Stefan, 2012, zv. A, pp. 337-340.
- Robert Bevec, Aleš Ude, "The acquisition of visual representation for object recognition by autonomous pushing", In: *RAAD 2012*, 21th International Workshop on Robotics in Alpe-Adria-Danube Region, 10-13 September 2012, Naples, Italy, [S. l.], ESA, = Edizioni Scientifiche e Artistiche, cop. 2012, pp. 156-161.
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- 8. Miha Deniša, Aleš Ude, "New movement primitives through graph search, optimized interpolation and statistical generalization", In: *RAAD 2012*, 21th International Workshop on Robotics in Alpe-Adria-

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- 11. Andrej Gams, Tadej Petrič, "Sklapljanje trajektorij za izvajanje dvoročnih nalog", In: Zbornik 15. mednarodne multikonference Informacijska družba - IS 2012, 8-12. oktober 2012, Ljubljana, Slovenia: zvezek A: volume A, (Informacijska družba), Marko Bohanec, ed., Matjaž Gams, ed., Dunja Mladenić, ed., Marko Grobelnik, ed., Marjan Heričko, ed., Urban Kordeš, ed., Maja Smrdu, ed., Olga Markič, ed., Zvezdan Pirtošek, ed., Jadran Lenarčič, ed., Leon Žlajpah, ed., Andrej Gams, ed., Vladislav Rajkovič, ed., Tanja Urbančič, ed., Mojca Bernik, ed., Ljubljana, Institut Jožef Stefan, 2012, zv. A, pp. 353-356.
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- 21. Tadej Petrič, Andrej Gams, Jan Babič, Tadej Debevec, Leon Žlajpah, "Control approaches for robotic knee exoskeleton device", In: *RAAD* 2012, 21th International Workshop on Robotics in Alpe-Adria-Danube Region, 10-13 September 2012, Naples, Italy, [S. l.], ESA, = Edizioni Scientifiche e Artistiche, cop. 2012, pp. 266-272.
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- 25. Daniela Zavec Pavlinič, Anica Hursa Šajatović, Igor B. Mekjavić, "Utjecaj osobne zaštitne opreme na zdravlje radnika", In: *Zbornik radova*, 4. Međunarodni stručno-znanstveni skup "Zaštita na radu i zaštita zdravlja", 19. - 22. rujan 2012, Zadar, Hrvatska, Jovan Vučinić, ed., Snježana Kirin, ed., Karlovac, Veleučilište u Karlovcu, = Karlovac University of Applied Sciences, 2012, pp. 701-706.
- 26. Daniela Zavec Pavlinič, Anica Hursa Šajatović, Igor B. Mekjavić, "Vrednovanje interventne odjeće za vatrogasce pomoću pozarne lutke", In: *Zbornik radova*, 4. Međunarodni stručno-znanstveni skup "Zaštita na radu i zaštita zdravlja", 19. - 22. rujan 2012, Zadar, Hrvatska, Jovan Vučinić, ed., Snježana Kirin, ed., Karlovac, Veleučilište u Karlovcu, = Karlovac University of Applied Sciences, 2012, pp. 707-712.

INDEPENDENT SCIENTIFIC COMPONENT PART OR A Chapter in a Monograph

- Jan Babič, "Biarticular actuation of robotic systems", In: *Robotic systems applications, control and programming*, Ashish Dutta, ed., Rijeka, InTech, cop. 2012, pp. 251-270.
- Andrej Gams, Tadej Petrič, Aleš Ude, Leon Žlajpah, "Performing periodic tasks: on-line learning, adaptation and synchronization with external signals", In: *The future of humanoid robots - research and applications*, Riadh Zaier, ed., Rijeka, InTech, cop. 2012, pp. 1-28.
- 3. Leon Žlajpah, Tadej Petrič, "Obstacle avoidance for redundant manipulators as control problem", In: *Serial and parallel robot manipulators - kinematics, dynamics, control and optimization*, Serdar Küçük, ed., Rijeka, InTech, cop. 2012, pp. 203-230.

PATENT APPLICATION

1. Igor Kovač, Borut Lenart, Bojan Nemec, Marko Scortegagna, Leon Žlajpah, *Humanoid torso mechanism*, P-201200214, Urad RS za intelektualno lastnino, 29.6.2012.

MENTORING

1. Fatih Bayazit, *On the asymptotic behavior of periodic evolution families on Banach spaces:* doctoral dissertation, Tübingen, 2012 (mentor Rainer Nagel; co-mentors Marjeta Kramar Fijavž, Britta Dorn).

DEPARTMENT OF SYSTEMS AND CONTROL

E-2

The department is engaged in the analysis, control and optimization of systems and processes. The activities of the department are focused on the research of new methods and algorithms for automatic control, the development of procedures and tools to support the design and construction of $control \ systems, the \ development \ of \ specific \ measurement \ and \ control \ modules, \ and \ the \ development$ and construction of complete systems for the control and supervision of machines, devices and industrial processes.

Basic and applied research

The basic and applied research in 2012 was devoted to three sub-areas: methodologies for analysis and control systems design; tools and building blocks for implementation; and applied research in the priority problem domains.

The sub-area methodologies for analysis and control systems design included three topics. The first topic addressed the modelling and identification of nonlinear and complex dynamical systems. The research in the dynamic systems modelling was directed towards the on-line training, analysis and application of Gaussian process models Head: for the modelling of static and the identification of dynamic systems. The application of modelling with Gaussian Dr. Vladimir Jovan process models of traffic, biological and environmental systems was pursued (Figure 1).



The second topic was (advanced) control. The developed methods for the implementation of the simplified explicit predictive controller were tested in pilot applications of liquid level control in a laboratory plant and the vertical stabilisation of the plasma position in the ITER tokamak fusion reactor model. We have shown the practical advantages enabled by systematic handling of constraints on the process signals, and successfully demonstrated control of the processes with fast dynamics, where a conventional predictive controller based on on-line optimisation is not useful due to the long computation time.

The third topic of interest was condition monitoring and fault diagnosis. A new robust method for bearings prognostics based on the concepts of the Jensen-Reny entropy, divergence and the complexity of vibrational signals

is proposed. The relationships between the entropy indices and the remaining useful life of the bearing are described by means of nonlinear dynamical systems. The approach is robust to incomplete information about the underlying operating conditions. With this algorithm our colleagues achieved the second-ranked result on a data challenge organized in the context of the international **IEEE PHM Conference.**

A key feature of modern condition monitoring systems in the ability to predict the remaining useful life of the system or its components. To achieve this, we focus on the

Figure 1: Uncertainty outcomes of the selected criterion for a given input action under input uncertainty. (Source: Water Research, 2012, vol. 46, no. 18, pp. 6121-6131)

development of system-identification algorithms for prognostics and health management (PHM). We have developed a prognostics algorithm, which relies on Gaussian Process models and applied it to bearings monitoring. More recently, we focused on the utilization of the Marginalized particle filtering framework for PHM.

We continued with the development of the prototype of a versatile low-cost platform (labelled MEMS-PHM) for the prognostics and health management of electro-mechanical drives. It relies on cutting-edge MEMS (microelectromechanical sensor) technologies. The hardware and software design of the underlying smart sensor node as well as the MEMS sensor prototype were almost completed. The first version of the MEMS-PHM platform was successfully implemented on a milling machine in the company LitostrojPower.

A part of the work, which is also related to condition monitoring, dealt with the problem of monitoring the water conditions inside a PEM fuel-cell stack. In 2012, we continued working on the diagnostics of flooding and drving inside PEM fuel cells with use of electrochemical impedance spectroscopy (EIS). In-house-developed measurement equipment made it possible to start dealing with the diagnostics of individual fuel cells inside a larger fuel-cell stack, which was before this unfeasible. The mentioned equipment was used for an experimental study,



which confirmed that the equipment itself is precise enough to perform the measurements the EIS requires. At the same time, valuable data was acquired for further research (Figure 2).

The sub-area tools and building blocks for implementation also included three parts. A method for the efficient control of under-damped systems has been developed. The method efficiently stabilizes systems in the open-loop and in the closed-loop configurations. In the frame of research dealing with tools and methodologies for process control software synthesis the work on a model-driven methodology for industrial process control software development



Figure 2: PEM fuel cells and measurement equipment during test operation

named MAGICS was continued. An empirical evaluation of this methodology was performed, which revealed an increase in productivity with savings between 18% and 33% of the total development effort and an improvement of the software quality due to the elimination of the code-generation errors. A new version of the development environment for this methodology was also developed (Figure 3).

In cooperation with the CONOT Center of Excellence Low Carbon Technologies we designed new components for fuel-cell-based power systems. In 2012 a diagnostic module for PEM fuel-cell-stack-based power units was developed as a low-cost solution for the on-line monitoring of each cell's voltage inside a stack. Besides the monitoring, the module provides the means for precise measurements of changes in the voltage of any individual cell inside a stack, which further enables the performance of the diagnostics of faults, such as cell flooding and membrane drying. The module is designed to perform measurements and data acquisition, further signal processing and diagnostics algorithm computation in real time (Figure 4).

Applied research in the priority problem domains was the third sub-area of our interest. In this frame a substantial part of our activities was devoted to the development of the specific control systems described below.

A numerically efficient version for signal de-noising based on an adaptive Kalman filter was implemented and assessed on plant data. The algorithm was applied to the pressure signal in order to improve the closed-loop control of the strip thickness in cold milling. The main idea is to manipulate the filter gain by means of the valve aperture. The work has been carried out in the frame of the international project PROBASENSOR.

We have implemented function blocks that enable the implementation of a simplified explicit predictive controller with constraints handling on industrial programmable-logic controllers in the IDR BLOK development environment, and have tested them in pilot applications.

Control of wastewater treatment plants is our traditional research area. A model of the entire Domžale-Kamnik wastewater treatment plant (WWTP) has been built, including both the water line and the sludge line. The model shows a relatively good agreement with the real-plant daily average measurements. It has been used for studying



Production control is also an important domain of our research work. The major problems in manufacturing today still relate to unexpected breakdowns and the degradation of product quality with no obvious reasons. In collaboration with the company Kolektor KFH, we have developed procedures for the automatic analysis of data form the production process. From these, the parameters that have a significant influence on the quality of the final product are determined. Additionally, the identified mathematical models are then used by the advanced production monitoring and control modules.

In the field of production control, we were continuing the evaluation of a concept of model-based production control. More emphasis was given to the modelling and production dynamics analysis, i.e., determination of the model structure, usage of modelling tools such as neural networks, fuzzy

logic and Petri nets. We were also designing a tool for production dynamic analysis to help us implement all the key activities necessary for holistic production control.

In recent years, a part of our work was focused on the area of fuel cells. In 2011 and 2012 we started cooperation on two newly 7th European projects FCGEN-Fuel Cell Based On-board Power Generation and FluMaBack-Fluid



Figure 3: Two engineering levels of the MAGICS methodology

Management component improvement for back-up fuel cell systems. The objective of the FCGEN project is the development and demonstration of an auxiliary power unit (APU) for trucks, which uses an auto-thermal reformer to produce hydrogen from fuel and a fuel-cell stack for electric energy production. The goal is the substitution of

low-efficiency main engine idling for covering electrical needs. Within the project both key components and system design will be further developed. The role of our group is the development of power conditioning, complete electronics and a control for all subsystems and for the integrated APU system. In the first half of 2012 the work mainly focused on the specification of the final process design of the APU system. Our group cooperated by making revising stages and providing solutions from the aspects of control and electric design. Additionally, the electrical APU layout has been designed and the APU load study performed. In the second half of 2012 the work was focused on determining the specifications for the APU's electrical layout and control system. In this context we determined the control concept, prepared a document with the specifications, developed part of the PLC software code and the HMI to monitor the entire process. In the FluMaBack project our group is responsible for improving the performance, cost efficiency and life time of essential balance of plant (BOP) components used in fuel-cellbased uninterruptable power back-up systems. In 2012 we started with the development of a PHM system for the condition monitoring of an air blower.



Figure 4: Diagnostic module for monitoring the fuel voltage of individual cells in a fuel-cell stack

Within the multidisciplinary project Ceracon-Integration and control of liquid fuel processor based on ceramic micro-systems which is financed by the European Space Agency we continued the development of the prototypes of critical components of the miniature size fuel reformer, which will serve as a source of hydrogen for miniature fuel cells. In 2012 we studied the efficiency of the reforming process as a function of the operating conditions and the type of catalyst.

R&D projects for industry and other users

A substantial part of the department's R&D activities for industry and other users is conducted within the Competence Centre for Advanced Control Technologies. In the second year of its operation, the first demonstration systems were developed, like an intelligent motor-drive valve, produced by the Danfoss Trata company, with an

embedded system for the automatic reduction of oscillations, and a wireless sensor network implemented for diagnostic and prognostic maintenance of machines at the Litostroj Power company. At other application domains, like production management with integrated models, the optimisation of energy consumption in buildings, the optimisation of gas production in bioreactors and the control of fusion reactors, the appropriate simulation environments were set-up with the preliminary design of advanced control algorithms.

As described below, an important part of our activities is also devoted to direct cooperations with various companies.

An important part of our activities in the past year was performed in close cooperation with the INEA company. One of the activities to mention was the development of a new version of the batch control software tool. In the area of the development of recipe-based batch process control package for the PLC platform (PLCbatch) the automatic generation of the phase logic software skeleton was realized. This tool significantly reduces the amount of the routine and repetitive development tasks and the resulting errors. A preliminary concept of the dynamic unit allocation was also realized, aimed at improving the flexibility of batch-control systems.

In the framework of the project for Danfoss, the hardware and the firmware for "heavy-duty" motor-drives is under development. A flow-controller has been developed, implemented and tested on a family of motor-driven



Figure 5: Diagnostic system for end quality control on the production line at Domel Electric Motors Suzhou Company Ltd.

valves. The department has been involved in the promotion of intelligent motor-driven valves and in user training. At Domel Electric Motors Suzhou Company Ltd., China, a new diagnostic system for the end quality control of electrical motors was completed in 2012 (Figure 5). The new system is the seventh in the series of similar, very successful diagnostic systems used in Domel.

Other projects

In 2012 the department has successfully concluded the tasks within the transnational project "Promoting Innovation in the Industrial Informatics and Embedded Systems Sector through Networking -13E". We have completed the final works regarding the main project outcomes that are the Strategic Research Agenda and Methodology Guideline for Innovation. In the final project phase our department has coordinated the final networking tasks and was actively involved in the promotion of the key project outcomes.

Educational and training activities

Some members of the department are giving lectures and practical courses at different faculties and universities: the Faculty of Electrical Engineering, University of Ljubljana, the Faculty of Logistics, University of Maribor, the University of Nova Gorica and the "Jožef Stefan" International Postgraduate School. They also act as supervisors of M.Sc. and Ph.D. students.

Some outstanding publications in the past year

- Boškoski, P., Juričić, D.: Fault detection of mechanical drives under variable operating conditions based on wavelet packet Rényi entropy signatures. Mech. syst. signal process., 2012, vol. 31, pp. 369–381
- Južnič-Zonta, Ž., Kocijan, J., Flotats, X., Vrečko, D.: Multi-criteria analyses of wastewater treatment bio-processes under an uncertainty and a multiplicity of steady states. Water research (Oxford). [Print ed.], 2012, vol. 46, no. 18, pp. 6121–6131
- 3. Perne, M., Šarler, B., Gabrovšek, F.: Calculating transport of water from a conduit to the porous matrix by boundary distributed source method. Eng. anal. bound. elem.. [Print ed.], 2012, vol. 36, no. 11, pp. 1649–1659
- Gerkšič, S., Pregelj, B.: Tuning of a tracking multi-parametric predictive controller using local linearan alysis. IET control theory & applications. [Print ed.], 2012, vol. 6, no. 5, pp. 1–11
- Glavan, M., Gradišar, D., Strmčnik, S., Mušič, G.: Production modelling for holistic production control. Simulation modelling practice and theory, 2013, vol. 30, pp. 1–20

Awards and appointments

- Damir Vrančić, Aleš Svetek: the Puh award for 2012, which is the highest state award for development achievements issued by the Ministry of Education, Science, Culture and Sport within the Zois awards - the state highest awards for scientific and research achievements. The Puh award was bestowed on our department members and the partners from Danfoss Trata for the invention of intelligent motor drives for valves
- Pavle Boškoski, Matej Gašperin, and Dejan Petelin were runners up in the IEEE PHM 2012 Prognostic Challenge (Data Challenge). They were invited to present their work at the 2012 IEEE International Conference on Prognostics and Health Management, Denver, Colorado, USA
- Juš Kocijan: Best paper award during the conference Applied Mathematics, Simulation, Modelling 2012, North Atlantic University Union NAUN with paper Dynamic GP models: an overview and recent developments, Vougliameni, Greece

The most important achievements in the past year

- 1. Puh Award for 2012, the highest national award for achievements in the field of development activities, was granted to Damir Vrancic and Ales Svetek for the invention of intelligent actuators for valves
- Implementation of an automatic diagnostic system for end quality control of electrical motors at Domel Electric Motors Suzhou Company Ltd., China. (Janko Petrovčič, Gregor Dolanc, Bojan Musizza, Stane Černe, Miroslav Štrubelj)
- 3. Pavle Boškoski, Matej Gašperin and Dejan Petelin were ranked in 2nd place among 20 teams on the IEEE PHM 2012 Prognostic Challenge for their solution for bearing's lifetime prediction. Their solutions were also presented as an invited lecture at the International Conference 2012 IEEE International Conference on Prognostics and Health Management, Denver, Colorado
- Darko Vrečko and Juš Kocijan published an article in the journal Water Research, which is the most eminent scientific journal in the field of water resources
INTERNATIONAL PROJECTS

- Completion of the Acroni controls; Project: 10AP100000-SIAC-J Plasmait Gmbh Dr. Gregor Dolanc
- 7. FP FCGEN: fuel cell based on-board power generation European Commission
- Dr. Boštjan Pregelj 3. 7. FP - FLUMABACK: Fluid management component improvement for back up fuel cell systems European Commission
- Dr. Pavle Boškoski
- I3E promoting innovation in the industrial informatics and embedded systems sectors through networking See Joint Technical Secretariat
 - Dr. Vladimir Jovan
- COST IC0702, SOFTSTAT: Combining soft computing techniques and statistical methods to improve data analysis solutions Cost Office
 - Cost Office
 - Prof. Juš Kocijan
- CERACON: Integration and control of liquid fuel processor based on ceramic microsystems
 - ÉSA/ESTEC
 - Dr. Gregor Dolanc
- COST IC0806, IntelliCIS: Intelligent monitoring, control, and security of critical infrastructure systems Cost Office
 - Dr. Nadja Hvala

R&D GRANTS AND CONTRACTS

 Identification and model analysis for dynamic systems control design with Gaussian process priors Prof. Juš Kocijan

VISITORS FROM ABROAD

- Prof. Giuseppe Ambrosino, Associazione Euratom-ENEA-CREATE, Dipartimento di Informatica e Sistemistica, Università di Napoli Federico II, Napoli, Italy, 16.–18. 1. 2012
- Dr. Gianmaria De Tommasi, Associazione Euratom-ENEA-CREATE, Dipartimento di Informatica e Sistemistica, Università di Napoli Federico II, Napoli, Italy, 16.–18. 1. 2012
- Daniel Toublant, scholarship IAESTE, Swansea University, Swansea, UK, 2. 7.–15. 8. 2012
 Henry Rafael Concepcion Gomez, Department of Telecommunications and Systems
- Henry Ratael Concepcion Gomez, Department of Telecommunications and Systems Engineering, Universitat Autonoma de Barcelona, Barcelona, Spain, 1. 8.–31. 11. 2012

- 2. Integrated diagnostic system for drive assemblies Prof. Đani Juričić
- Prognostics and health management of mechanical drives based on novel MEMS sensor networks Prof. Dani Iuričić
- Modeling and control of wastewater treatment plants for improving the effluent quality and energy effective operation Dr. Darko Vrečko
- Advanced model based procedures for product quality control and management in complex production processes
- Prof. Đani Juričić 6. Simplified explicit predictive controller Prof. Stanislav Strmčnik
- Probasensor: EUROSTARS; Probalistic bayesian soft sensor a tool for on-line estimation of the key process variable in cold rolling mills
- Prof. Đani Juričić
 8. Competence centre for advanced control technologies: CC ACT Asst. Prof. Damir Vrančić

RESEARCH PROGRAM

 Program systems and control Prof. Đani Juričić

NEW CONTRACTS

- Prognostics and health management of mechanical drives based on novel mems sensor networks
- Domel, d. o. o. Prof. Đani Juričić
- R&D Activities in the frame of the KC STV sub-projects No. 1.1, No. 1.2, and No. 4.2. Inea, d. o. o. Giovanni Godena, M. Sc.
- 5. Prof. Vesna Mandič, University of Kragujevac, Kragujevac, Serbia, 23. 7. 2012
- Prof. Milentije Stefanović, University of Kragujevac, Kragujevac, Serbia, 23. 7. 2012
- 7. Prof. Dragan Milosavljević, University of Kragujevac, Kragujevac, Serbia, 23. 7. 2012
- 8. Dr. Elisabet Capon Garcia, ETH, Zürich, Switzerland, 22. 10. 2012
- 9. Dr. Edrisi Munoz Mata, CIMAT, Zacatecas, Mexico, 22. 10. 2012

STAFF

Researchers

- 1. Dr. Gregor Dolanc
- 2. Dr. Samo Gerkšič
- 3. Giovanni Godena, M. Sc.
- 4. Dr. Dejan Gradišar
- 5. Dr. Nadja Hvala
- 6. Dr. Vladimir Jovan, Head
- 7. Prof. Đani Juričić
- 8. Dr. Gregor Kandare, left 18.06.12
- 9. Prof. Juš Kocijan
- 10. Dr. Janko Petrovčič
- 11. Prof. Stanislav Strmčnik
- Asst. Prof. Damir Vrančić
 Dr. Darko Vrečko

Postdoctorial associates

- 14. Dr. Pavle Boškoski
- 15. Dr. Matej Gašperin

- Dr. Marko Nerat
 Dr. Boštjan Pregelj
 Postgraduates
 Andrej Debenjak, B. Sc.
 Miha Glavan, B. Sc.
 Dr. Tomaž Lukman
- 22. Jernej Mrovlje, M. Sc., left 01.11.12
- 23. Dr. Matija Perne

16. Dr. Bojan Musizza

- 24. Dejan Petelin, B. Sc.
- 25. Aleš Svetek, M. Sc. Technical officers
- 26. Stanislav Černe, B. Sc.
- 27. Primož Fajdiga, B. Sc.
- Technical and administrative staff
- Maja Janežič, B. Sc.
 Miroslav Štrubelj

BIBLIOGRAPHY

ORIGINAL SCIENTIFIC ARTICLE

- 1. Darko Belavič, Marko Hrovat, Gregor Dolanc, Marina Santo-Zarnik, Janez Holc, Kostja Makarovič, "Design of LTCC-based ceramic structure for chemical microreactor", *Radioengineering (Prague)*, vol. 21, issue 1, pp. 195-200, 2012.
- Pavle Boškoski, Đani Juričić, "Fault detection of mechanical drives under variable operating conditions based on wavelet packet Rényi entropy signatures", *Mech. syst. signal process.*, vol. 31, pp. 369-381, 2012.
- Andrej Fabjan, Bojan Musizza, Fajko Bajrović, Marjan Zaletel, Martin Štrucl, "The effect of the cold pressor test on a visually evoked cerebral blood flowvelocity response", *Ultrasound med. biol.*, vol. 38, no. 1, pp. 13-20, Jan. 2012.
- 4. Samo Gerkšič, Boštjan Pregelj, "Tuning of a tracking multi-parametric predictive controller using local linear analysis", *IET control theory & applications*, vol. 6, no. 5, pp. 1-11, 2012.
- Karina Gibert, Dante Conti, Darko Vrečko, "Assisting the end-user in the interpretation of profiles for decision support, An application to wastewater treatment plants", *Environ. Eng. Manag. J. (Print)*, vol. 11, no. 11, pp. 931-944, 2012.
- Miha Glavan, Matej Gašperin, Matej Vidmar, Maks Tuta, Stojan Kokošar, Đani Juričić, Andrej Brložnik, "Analiza proizvodnih podatkov za nadzor in upravljanje kvalitete izdelkov", *Ventil (Ljubl.)*, vol. 18, no. 5, pp. 396-402, nov. 2012.
- Živko Južnič-Zonta, Juš Kocijan, Xavier Flotats, Darko Vrečko, "Multicriteria analyses of wastewater treatment bio-processes under an uncertainty and a multiplicity of steady states", *Water res. (Oxford)*, vol. 46, no. 18, pp. 6121-6131, 2012.
- Gregor Kandare, Nadja Hvala, Marijan Vidmar, "Vključevanje večjih rezidenčnih in manjših industrijskih uporabnikov v pametna omrežja", *Ventil (Ljubl.)*, vol. 18, no. 3, pp. 210-214, jun. 2012.
- 9. Gregor Kandare, Daniel Viúdez-Moreiras, Félix Hernández-del-Olmo, "Adaptive control of the oxidation ditch reactors in a wastewater treatment plant", *Int. j. adapt. control signal process.*, vol. 26, no. 10, pp. 879-989, 2012.
- 10. Bojan Musizza, Fajko Bajrović, Janko Petrovčič, Aneta Stefanovska, Samo Ribarič, "Fluctuations and interactions between brain waves during deep and shallow anesthesia", *Fluctuation and noise letters*, vol. 11, no. 1, pp. 1240018-1-1240018-12, 2012.
- 11. Marko Nerat, "Copper-indium-gallium-selenide (CIGS) solar cell with localized back contacts for achieving high performance", *Sol. energy mater. sol. cells*, vol. 104, pp. 152-158, 2012.
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- 13. Gabrijel Peršin, José Salgueiro, Jože Vižintin, Đani Juričić, "A system for automated online oil analysis", *Insight (Northamp.)*, vol. 54, no. 8, pp. 428-432, 2012.
- 14. Jan Přikryl, Juš Kocijan, "Stochastic analysis of a queue length model using a graphical processing unit", *Trans. Transp. Sci. (Print)*, vol. 5, no. 2, pp. 55-62, 2012.
- 15. Edvin Raubar, Damir Vrančić, "Anti-sway system for ship-to-shore cranes", *Stroj. vestn.*, vol. 58, no. 5, pp. 338-344, 2012.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION (INVITED LECTURE)

- 1. Pavle Boškoski, Matej Gašperin, Dejan Petelin, "Bearing fault prognostics based on signal complexity and Gaussian process models", In: *PHM*'12, 2012 IEEE International Conference on Prognostics and Health Management, June 18-21, 2012 - Denver, Colorado, Denver, IEEE, 2012, 8 pp.
- 2. Đani Juričić, Pavle Boškoski, Matic Ivanovič, Janko Petrovčič, Bojan Musizza, Matej Gašperin, Jože Vižintin, "Sprotni nadzor stanja industrijskih pogonov", In: Zbornik predavanj Posvetovanja o tribologiji, hladilno mazalnih sredstvih in tehnični diagnostiki, Posvetovanje o tribologiji, hladilno mazalnih sredstvih in tehnični diagnostiki = Conference on Tribology, Metal Working Fluids and Technical Diagnostics [tudi] SLOTRIB 2012, Ljubljana, Slovenija, 15.

november 2012, Jože Vižintin, ed., Marko Sedlaček, ed., Ljubljana, Slovensko društvo za tribologijo, = Slovenian Society for Tribology, 2012, pp. 55-65.

- 3. Juš Kocijan, "Dynamic GP models: an overview and recent developments", In: Recent researches in applied mathematics and economics: proceedings of the 6th International Conference on Applied Mathematics, Simulation, Modelling, (ASM'12), proceedings of the 6th International Conference on Management, Marketing and Finances, (MMF'12), March 7-9, 2012, Tsutomu Kambe, ed., Cornelia A. Bulucea, ed., Charalampos Arapatsakos, ed., [S. I.], WSEAS Press, = World Scientific and Engineering Academy and Society, 2012, pp. 38-43.
- 4. José Salgueiro, Gabrijel Peršin, Jože Vižintin, Đani Juričić, "A system for on-line oil analysis", In: Zbornik predavanj Posvetovanja o tribologiji, hladilno mazalnih sredstvih in tehnični diagnostiki, Posvetovanje o tribologiji, hladilno mazalnih sredstvih in tehnični diagnostiki = Conference on Tribology, Metal Working Fluids and Technical Diagnostics [tudi] SLOTRIB 2012, Ljubljana, Slovenija, 15. november 2012, Jože Vižintin, ed., Marko Sedlaček, ed., Ljubljana, Slovensko društvo za tribologijo, = Slovenian Society for Tribology, 2012, pp. 81-96.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- 1. Darko Belavič, Marko Hrovat, Gregor Dolanc, Kostja Makarovič, Marina Santo-Zarnik, Janez Holc, "Design of an LTCC structure for a microceramic combustor", In: *Proceedings*, IMAPS/ACerS, 8th International Conference and Exhibition on Ceramic Interconnect and Ceramic Microsystems Technologies (CICMT 2012), April 16-19, 2012, Erfurt, Germany, [S. l.], International Microelectronics and Packaging Society, 2012, pp. 288-293.
- Pavle Boškoski, Đani Juričić, "Rényi entropy based statistical complexity analysis for gear fault prognostic sunder variable load", In: Condition monitoring of machinery in non-stationary operations: proceedings of the Second International Conference Condition Monitoring of Machinery in Non-stationnary Operations, 2012, [March 26-28, 2012, Hammamet, Tunisia], Tahar Fakhfakh, ed., Haidelberg [etc.], Springer, 2012, pp. 25-32.
- 3. Andrej Debenjak, "Diagnostika sistemov z gorivnimi celicami in izboljšanje njihovega delovanja", In: *Zbornik*, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 119-124.
- 4. Andrej Debenjak, Vladimir Jovan, Janko Petrovčič, Matej Gašperin, Boštjan Pregelj, "An assessment of water conditions in a PEM fuel cell stack using electrochemical impedance spectroscopy", In: Proceedings of IEEE 2012 [3rd Annual] Prognostics and System Health Management Conference, (PHM-2012 Beijing), 23-25 May 2012, Beijing, China, Suzanne Zhang, ed., Rui Kang, ed., Michael Pecht, ed., Danvers, IEEE, 2012, pp. MU3036-1-MU3036-6.
- 5. Andrej Debenjak, Boštjan Pregelj, Matej Gašperin, Janko Petrovčič, "Koncept diagnostike sistemov s PEM gorivnimi celicami", In: *Vir* znanja in izkušenj za stroko: zbornik foruma, Industrijski forum IRT, Portorož, 11. in 12. junij 2012, Tomaž Perme, ed., Darko Švetak, ed., Škofljica, Profidtp, 2012, pp. 217-222.
- Matej Gašperin, Đani Juričić, Pavle Boškoski, "Prediction of the remaining useful life: an integrated framework for the model estimation and failure prognostics", In: *PHM*'12, 2012 IEEE International Conference on Prognostics and Health Management, June 18-21, 2012 - Denver, Colorado, Denver, IEEE, 2012, 8 pp.
- 7. Samo Gerkšič, Gianmaria De Tommasi, "Vertical control of ITER plasma using explicit model predictive control", In: *SOFT 2012*, 27th Symposium on Fusion Technology, September 24-28, 2012, Liège, (Belgium), [S. l., s. n.], 2012.
- 8. Miha Glavan, Matej Gašperin, Matej Vidmar, Maks Tuta, Stojan Kokošar, Đani Juričić, Andrej Brložnik, "Iskanje vplivnih parametrov v kompleksnih proizvodnih procesih", In: *Zbornik enaindvajsete mednarodne Elektrotehniške in računalniške konference ERK 2012, 17.* 19. september 2012, Portorož, Slovenija, (Zbornik ... Elektrotehniške in računalniške konference ERK ...), Baldomir Zajc, ed., Andrej Trost, ed.,

Ljubljana, IEEE Region 8, Slovenska sekcija IEEE, 2012, zv. A, pp. 211-214.

- 9. Miha Glavan, Dejan Gradišar, "Controllability of holistic production control", In: *Proceedings CD: IEEE-ICIT'12, International Conference on Industrial Technology, 19-21 March, 2012, Athens, Greece*, [S. l.], IEEE, 2012, pp. 65-70.
- Dejan Gradišar, Miha Glavan, "Input variable selection algorithms for HPC", In: Proceedings CD: IEEE-ICIT'12, International Conference on Industrial Technology, 19-21 March, 2012, Athens, Greece, [S. l.], IEEE, 2012, pp. 71-76.
- Dejan Gradišar, Ingrid Petrič, "Ključni kazalniki učinkovitosti za proizvodnjo", In: Zbornik enaindvajsete mednarodne Elektrotehniške in računalniške konference ERK 2012, 17.-19. september 2012, Portorož, Slovenija, (Zbornik ... Elektrotehniške in računalniške konference ERK ...), Baldomir Zajc, ed., Andrej Trost, ed., Ljubljana, IEEE Region 8, Slovenska sekcija IEEE, 2012, zv. A, pp. 169-172.
- 12. Nadja Hvala, Darko Vrečko, Meta Levstek, Cirila Bordon, "Uporaba matematičnih modelov pri nadgradnji čistilnih naprav", In: Zbornik referatov: [simpozij z mednarodno udeležbo], Simpozij z mednarodno udeležbo Vodni dnevi 2012, Portorož, 16.-18. oktober 2012, Milenko Roš, ed., Ljubljana, Slovensko društvo za zaščito voda, 2012, pp. 37-48.
- 13. Matic Ivanovič, Pavle Boškoski, Đani Juričić, Jože Vižintin, "An environment for efficient design and implementation of condition monitoring systems for mechanical drives", In: *CM 2012/MFPT 2012*, The 9th International Conference on Condition Monitoring and Machinery Failure Prevention Technologies, 12-14 June 2012, London, UK, Northampton, The British Institute of NT, 2012, 11 pp.
- 14. Matic Ivanovič, Đani Juričić, "Prototip sistema za sprotni nadzor stanja industrijske opreme", In: Zbornik, 4. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 4th Jožef Stefan International Postgraduate School Students Conference, 25. maj 2012, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Boštjan Kaluža, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2012, pp. 131-136.
- 15. Đani Juričić, Pavle Boškoski, Matej Gašperin, Dejan Petelin, "Robust diagnosis and prognosis based on entropy indices", In: *MPMM 2012 proceedings*, The 2nd International Conference on Maintenance Performance Measurement and Management, 12th-13th September 2012, Sunderland, UK, D. Galar, ed., Sunderland, University of Sunderland, 2012, 6 pp.
- P. B. de Moura Oliveira, Damir Vrančić, J. Boaventura Cunha, "Posicast PID control of oscillatory systems", In: *Controlo' 2012*, 10th Portuguese Conference on Automatic Control, 16-18 July 2012, Funchal, Madeira Island, Portugal, Madeira, Associação Portuguesa de Controlo Automático, 2012, pp. 27-32.
 Igrnej Mrovlje, Damir Vrančić, "Automatic detection of the truck
- 17. Jernej Mrovlje, Damir Vrančić, "Automatic detection of the truck position using stereoscopy", In: *Proceedings CD: IEEE-ICIT'12, International Conference on Industrial Technology, 19-21 March, 2012, Athens, Greece*, [S. l.], IEEE, 2012, pp. 766-770.
- 18. Jernej Mrovlje, Damir Vrančić, "Učinkovitost tabeliranega bilinearnega modela distorzije", In: Zbornik enaindvajsete mednarodne Elektrotehniške in računalniške konference ERK 2012, 17.-19. september 2012, Portorož, Slovenija, (Zbornik ... Elektrotehniške in računalniške

konference ERK ...), Baldomir Zajc, ed., Andrej Trost, ed., Ljubljana, IEEE Region 8, Slovenska sekcija IEEE, 2012, zv. B, pp. 165-168.

- 19. Gabrijel Peršin, José Salgueiro, Jože Vižintin, Đani Juričić, "Mechanical systems fault diagnosis in variable operating conditions by feature modelling", In: *CM 2012/MFPT 2012*, The 9th International Conference on Condition Monitoring and Machinery Failure Prevention Technologies, 12-14 June 2012, London, UK, Northampton, The British Institute of NT, 2012, 13 pp.
- 20. José Salgueiro, Gabrijel Peršin, Jože Vižintin, Đani Juričić, "A system for automated on-line oil analysis", In: *CM 2012/MFPT 2012*, The 9th International Conference on Condition Monitoring and Machinery Failure Prevention Technologies, 12-14 June 2012, London, UK, Northampton, The British Institute of NT, 2012, 13 pp.
- Damir Vrančić, P. B. de Moura Oliveira, "Design of feedback control for underdamped systems", In: *PID'12*, IFAC Conference on Advances in PID Control, March 28-30, 2012, Brescia, (Italy), Ramon Vilanova, ed., Antonio Visioli, ed., [S. I.], IFAC, 2012, 6 pp.
 Damir Vrančić, P. B. de Moura Oliveira, "Underdamped second-order
- 22. Damir Vrančić, P. B. de Moura Oliveira, "Underdamped second-order systems overshoot control", In: *PID'12*, IFAC Conference on Advances in PID Control, March 28-30, 2012, Brescia, (Italy), Ramon Vilanova, ed., Antonio Visioli, ed., [S. l.], IFAC, 2012, 6 pp.

INDEPENDENT SCIENTIFIC COMPONENT PART OR A

CHAPTER IN A MONOGRAPH

- Dejan Gradišar, Gašper Mušič, "Automated Petri-net modelling for batch production scheduling", In: *Petri nets - manufacturing and computer science*, Pawel Pawlewski, ed., Rijeka, InTech, cop. 2012, pp. 3-26.
- Damir Vrančić, "Magnitude optimum techniques for PID controllers", In: Introduction to PID controllers: theory, tuning and application to frontiers areas, Rames C. Panda, ed., Rijeka, InTech, cop. 2011, pp. 75-102.

MENTORING

- 1. Tomaž Lukman, A methodology for the development of industrial process control software: doctoral dissertation, Maribor, 2012 (mentor Marjan Heričko; co-mentor Stanko Strmčnik).
- 2. Matija Perne, *Modelling speleogenesis in transition from pressurised to free surface flow:* doctoral dissertation, Nova Gorica, 2012 (mentors Franci Gabrovšek, Georg Kaufmann).
- 3. Miha Menard, *Design and implementation of control structures for industrial processes:* master's thesis, Ljubljana, 2012 (mentor Gregor Klančar; co-mentor Damir Vrančić).
- 4. Jernej Mrovlje, *Distortion impact on the objects's location calculated by using stereoscopic images:* master's thesis, Ljubljana, 2012 (mentor Damir Vrančić).
- 5. Aleš Urdih, Analysis of recent electric-generator patents for small wind turbines: master's thesis, Nova Gorica, 2012 (mentor Juš Kocijan).

ARTIFICIAL INTELLIGENCE LABORATORY

The Artificial Intelligence Laboratory (http://ailab.ijs.si/) is concerned mainly with research and development in information technologies, with an emphasis on artificial intelligence. The main research areas are the following: data analysis with an emphasis on text, web and cross-modal data, scalable real-time data analysis, machine learning, analysis and modelling of large networks, visualization of complex data, semantic technologies, language technologies, reasoning methods and knowledge management. The Artificial Intelligence Laboratory has employees and students with an international background and with expertise in different areas of artificial intelligence. In addition to having their research results published in international publications, they have also developed several software tools for multimodal data analysis. Some of these tools are: Text-Garden, a suite of text-mining tools; OntoGen (http://ontogen.ijs.si/), a tool for ontology learning; Document-Atlas (http://docatlas.ijs.si/), a tool for complex visualization; Atlas of Slovenian Science (http://scienceatlas.ijs.si/), a web portal for analyzing the scientific community; AnswerArt (http:// answerart.net/), a system for semantic search on large databases (AFSA, OpenCyc, WordNet); Head: Enrycher (http://enrycher.ijs.si/), a system for semantic enrichment of textual data; SearchPoint Prof. Dunja Mladenić (http://searchpoint.ijs.si/), a portal for visual and contextualized web browsing; OntoPlus, a methodology for semi-automatic ontology extension; Contextify (http://contextify.net/), a tool for contextualized e-mail and contact management; NewsFeed (http://newsfeed.ijs.si/), a clean, continuous, real-time aggregated stream of semantically enriched news articles from RSS-enabled sites across the world. The laboratory's strategy is to combine scientific excellence and strong collaboration with industry, and to transfer research results into real-world business environments.



In the past 10 years, members of the Artificial Intelligence Laboratory successfully completed 27 EU projects, of which 4 were concluded in 2012. In addition, we were involved in another 14 EU 7FP projects in 2012, including

3 networks of excellence covering three complementary research areas: statistical data modelling and machine learning, language technologies, and semantic technologies. Among the national projects we can emphasize our involvement in two competence centres and three national application projects.

In the area of statistical data modelling and machine learning, our activities within PASCAL2 (Pattern Analysis, Statistical Modelling and Computational Learning 2), an EU network of excellence, were mainly on investigating class imbalance in high-dimensional data related to the hubness phenomenon and hubness'aware shared neighbour distance for k-nearest neighbour classification. As a part of our activities in PASCAL2 Harvest we have concluded the project LaVie (user recommendation for related lectures on VideoLectures.NET), that will go

live on the VideoLectures.NET portal in 2013. We have concluded work on the ESC (European Security Challenge) EU project, where we have defined the rules and guidelines for organizing competitions on the topic of security, intended for promoting the development and evaluation of technology-based machine learning, such as robotics, computer system security and computer vision. In the XLike (Cross-lingual Knowledge Extraction) EU FP7 project coordinated by our department, we have developed and validated the first prototype, which encompasses multilingual linguistic processing, crosslingual semantic annotation and cross-lingual document linking. Significant advancements were made in the area of cross-lingual document linking by developing methods which can scale to 50 languages, including minority languages with limited training-corpora availability. The prototype was evaluated by the two use-case partners: (a) Bloomberg for recommending

In 2012 we started the coordination of three EU projects (XLike, TOPOSYS, NRG4Cast) and began an additional four EU projects



Figure 1: The prototype for cross-lingual news analysis developed in the XLike project.

local news content to German, Spanish, French and Italian audiences, and (b) the Slovenia Press Agency to improve the process of monitoring Slovenian entities in foreign news media. We started with the EU FP7 project Sophocles (Self-Organised information PrOcessing, CriticaLity and Emergence in multilevel Systems), on developing mathemati-



Figure 2: ArchiveExplorer visualizing the New York Times news about Princes Diana.

cal and computational formalisms for information processing in multi-level systems. We started with the EU FP7 project TOPOSYS (http://toposys.org/), in the area of the dynamics of multilevel complex systems.

Our work on text and network analysis connects language technologies, machine learning, semantic technologies and cross-modal data-processing methods. Within the EU 7FP project ALERT (active support and real-time coordination based on event processing in FLOSS development) we implemented tools and methods for the monitoring, analysis and semantic annotation of all the data generated in information channels used in software development (issue-tracking systems, source-code management systems, forums and mailing lists). Using the processed information we are able to provide a semantic search across all information channels, identify duplicated bug reports, suggest developers to fix an issue, identify issues potentially created by a particular developer, etc. Within Planet Data (Intelligent Information Management), an EU network of excellence, we have developed ArchiveExplorer, a system for the analysis of semantically enriched texts through time including extracting social context and relationships from text corpora. In collaboration with the Institute's Communication Systems Department (E6) we have developed an automatic meta-data collection and annotation system which automatically collects context information for individual sensor nodes, then annotates them and stores them in a triple store on the server side (incorporated in the Videk demo application, which enables intelligent monitoring of the environmental sensor data). In addition Videk was extended by a natural language generation module which relies on the semantic representation of the meta-data in ResearchCyc. Within Slovenian Science Atlas, a national project, we extended our system for the search and visualization of research collaboration and competences of the scientists working in Slovenia to emphasize the difference between business and research collaborations. In

RENDER (Reflecting Knowledge Diversity), an EU 7FP project, we have developed a Diversity Mining Toolkit which encompasses fact extraction and opinion mining applications working on a live stream of news articles. The Toolkit is extensively used on real-world data (1) to aid Wikipedia editors by providing up-to-date ranked news articles for Wikipedia articles, (2) to analyse sentiment in Twitter data for Telefonica, (3) as a part of a Google interactive tool which allows users to browse and summarize news articles from different perspectives.

In the area of **language technologies**, our main contributions in the project METANet (Net Technologies for the Multilingual European Information Society) (FP7 Network of Excellence on Linguistics: http://www.meta-net.eu/)

In 2012 we won the second-best demo award at the ESWC Conference on the Semantic Web.

were (a) covering a road-map for future EU research programs in linguistics (http://www.meta-net.eu/vision/reports/meta-net-sra-version_1.0.pdf) in the area of Social Intelligence and e-Participation and (b) preparing White book on "The Slovene Language in the Digital Age" (http://www.

meta-net.eu/whitepapers/volumes/slovene) covering all the language resources for Slovenian language. Within MultilingualWeb (Advancing the Multilingual Web), an EU 7FP project, we worked on establishing the community for the standards and concrete examples of tools that support the construction, localization and use of multilingual web data. We also participated in the organization of events that encourage the standardization of multilinguality on the web. By performing in the role of natural language processing providers, we have promoted the use of our multilingual semantic annotation tool Enrycher. As part of our activity in the EU FP7 project LT-Web, we are participating in the standardization process in the role of natural language processing service providers. The new MultilingualWeb-LT (Language Technology) W3C Working Group will develop standard ways to support the (automatic and manual) translation and adaptation of web content to local needs, from its creation to its delivery to end users. For this purpose, we have promoted the use of our multilingual semantic annotation tool Enrycher as a reference implementation of the ITS2.0 standard (Internationalization Tag Set). Within Communication in Slovene, a national project, we contributed to the resolution on the national program for language policies.

Our work in the area of **semantic technologies** led not only to the research results, but also to an integration of new methods into the prototype systems. We successfully concluded our work within the EU project ENVISION (ENVIronmental Services Infrastructure with ONtologies) focused on the analysis of stream data and development of the methods for the semantic enrichment of the sensor data, where we have also addressed a problem of supporting complex event rule generation and validation on environmental data. We have also developed methods

Jure Leskovec won an award for his current work in the area of information society at the IS-2012 Conference

for measuring concept similarity in ontologies which do not use additional corpora aside from ontology itself, where the experimental evaluation was performed on OpenCyc ontology and on the WordNet lexical database. We also developed a framework for acquiring semantic sensor descriptions with the help of mobile devices (contextual metadata of sensors such as

location and the surrounding environment) and a framework for the semantic enrichment of sensor descriptions and measurements. In addition, we have developed an approach to environmental data mining and applied it to a problem of mining data from a public bicycle system including environmental information on weather, bicyclestation location, time of the day and day of the week, and the number of bicycles at each hour at each station.

Knowledge management includes research and development by using methods and tools from a broader AI area in the real business settings. In 2012 we started three new FP7 projects. The aim of NRG4Cast (Energy Forecasting) is the development of real-time management, analytics and forecasting services for energy-distribution networks in urban/rural communities. MobiS (Personalized Mobility Services for energy efficiency and security through

advanced Artificial Intelligence techniques) deals with a new concept and the solution of a federated, customized and intelligent mobility platform by applying novel Future Internet technologies and Artificial Intelligence methods that will monitor, model and manage the urban mobility complex network of people, objects, natural, social and business environment in real

Blaž Fortuna had an invited talk at the AAAI Workshop on Intelligent Techniques for Web Personalization and Recommendation systems

time. Mediamixer (Community set-up and networking for the remixing of online media fragments) is looking at the value and use of the fragmented media content. It will set up and sustain a community of video producers, hosters and redistributors who will be supported in the adoption of semantic multimedia technology in order to build a European market for media fragment re-purposing and re-selling.

The Artificial Intelligence Laboratory puts special emphasis on the promotion of science. We have successfully concluded the national project Youth Network of Research Values (SM-RIS) as a part of which we have organized a

touring exhibition about female PhD graduates from the area of computer science in Slovenia. We have been organizing this exhibition since 2006, thereby promoting the role of women in science (http://ScienceWithArt. ijs.si/). We have successfully concluded the EU project GENDERA (Gender Debate in the European Research Area), contributing to the recommendations addressing gender equality in research organizations and a presentation for the promotion of gender equality in research organizations at the European Conference on Gender and Innovation (http://videolectures.net/ gender innovation2012 stuttgart/). Our work within SIS-Catalyst (Children as Change Agents for Science in Society), a 7FP project in social sciences, was focused on the analysis of data regarding the participation of young people at scientific events, exhibitions, workshops and summer schools that specifically target the youth. Our activities on TransLectures (Transcription and Translation of Video Lectures), an EU 7FP project, where we collaborate with the Centre for Knowledge Transfer in Information Technologies (CT3) on the automated subtitling and translating of video recordings, were focused on the architectural adaptation of case studies (VideoLectures.NET and Matterhorn) and the platform integration, where we have made excellent Figure 3: A system for the analysis of sensor data developed in the progress, also in terms of intelligent interaction with the user. Together with Envision project. CT3 we continued to use the videolectures.NET portal to promote artificial



intelligence, the Institute, and Slovenian research in general. Our laboratory is also the main organizer and supporter of the annual national ACM Computer Science Competition for secondary-school students; this year, more than 300 students participated in the competition.

In 2012 we were very actively involved in submitting new project proposals, particularly within the 7th framework programme. Once again we were very successful in this, winning five new projects, and also being appointed

as coordinators of two of them. We continue with our successful efforts to include Slovenian industry into the European research area; the list of 16 companies participating in EU projects has been extended by two. In total, we invited 8 Slovenian businesses to participate with us in the EU project proposals submitted in 2012.

Some outstanding publications in the past year

- 1. Chazal, F., Škraba, P., Patel, A.: Computing well diagrams for vector fields on R[sup]n. Appl. math. lett. [Print ed.], 2012, vol. 25, no. 11, pp. 1725-1728
- 2. Tomašev, N., Radovanović, M., Mladenić, D., Ivanović, M.: Hubness-based fuzzy measures for high-dimensiona k-nearest neighbor classification. Int. j. mach. learn. cybern. (Print), 2012, pp. 14
- Dali, L., Fortuna, B., Tran, T., Mladenić, D.: Query-independent learning to rank for RDF entity search. Lect. 3. notes comput. sci., 2012, INCS 7295, pp. 486-513
- Fortuna, C., Grobelnik, M.: From sensors to real-time analytics. Elektrotehniški vestnik. [Slovenska tiskana 4. izd.], 2012, vol. 79, no. 5, pp. 273-277.

Dunja Mladenić had an invited lecture at the 4th International Conference on Information Technologies and Information society.



5. Škrbec, J., Grobelnik, M., Fortuna, B.: Exploring history through newspaper archives : presented at the extended semantic web conference, ESWC 2012, Heraklion, Crete, Greece, 27.-30. 5. 2012

Organization of conferences, congresses and meetings

- 1. Project meeting 7. OP XLIKE, Bled, 18.-20. 1. 2012
- 2. Project meeting 7. OP RENDER, Dubrovnik, Croatia, 4.-6. 7. 2012
- 3. Conference on Data Mining and Data Warehouses 2012, Ljubljana, 8. 10. 2012
- 4. Conference on 100 YEARS OF ALAN TURING AND 20 YEARS OF SLAIS, Ljubljana, 11. 10. 2012
- 5. Project meeting 7. OP TOPOSYS, Ljubljana, 28.–31. 10. 2012
- 6. Project hackatton 7. OP XLIKE, Ljubljana, 4.-7. 11. 2012
- 7. Project meeting 7. OP NRG4Cast, Ljubljana, 13.–14. 12. 2012

INTERNATIONAL PROJECTS

- 7. FP PASCAL2: Pattern analysis, statistical modelling and computational learning 2 European Commission Prof. Dunia Mladenić
- 7. FP GENDERA: Gender debate in the European research area European Commission
- Prof. Dunja Mladenić
 7. FP ENVISION: Environmental services infrastructures with ontologies European Commission
- Prof. Dunja Mladenić
- 4. 7. FP MetaNET: Technologies for the multilingual European information society European Commission
- Marko Grobelnik 5. 7. FP - RENDER: Reflecting knowledge diversity European Commission
- Prof. Dunja Mladenić 6. FP – PlanetData
- European Commission Marko Grobelnik
- FP ALERT: Active support and real-time coordination based on event processing in Open Source software development European Commission
- Prof. Dunja Mladenić
- FP SiS CATALYST: Children as change agents for the future of science in society European Commission Prof. Dunja Mladenić
- 9. 7. FP transLectures: Transcription and translation of video lectures European Commission
- Prof. Dunja Mladenić 10. 7. FP - LT-Web: Language technology in the web
- European Commission Prof. Dunja Mladenić
- 7. FP MEDIAMIXER: Community set-up and networking for the remixing of online media fragments European Commission
- Marko Grobelnik
- 7. FP MobiS: Personalized mobility services for energy efficiency and security through advanced artificial intelligence techniques European Commission
- Marko Grobelnik
- 7. FP ESC: European security challenge European Commission Marko Grobelnik
- 14. 7. FP X-Like: Cross-lingual knowledge extraction European Commission
 - Marko Grobelnik

VISITORS FROM ABROAD

- 1. Evan Sandhaus, New York Times, New York, USA, 13.-20. 1. 2012
- Swaran Lata, Department of Information Technology, Government of India, India, 17.–21. 1. 2012
- 3. Abe Hsuan, Irwin & Hsuan LLP, New York, USA, 18.-20. 1. 2012
- 4. Michael Witbrock, Cycorp Europe, d.o.o., Ljubljana, Slovenia, 18.-20. 1. 2012
- 5. Juanzi Li, Tsinghua University, Beijing, China, 17.–20. 1. 2012
- 6. John Davies, British Telecom, London, UK, 14.–17. 2. 2012
- 7. Abe Hsuan, Irwin & Hsuan LLP, New York, USA, 6.-13. 7. 2012
- 8. Michael Witbrock, Cycorp Europe, d.o.o., Ljubljana, Slovenia, 6.-13. 7. 2012
- 9. Rok Sosič, Stangord University, Palo Alto, USA, 2.-24. 8. 2012

- 7. FP TOPOSYS: Topological complex system European Commission Dr. Primož Škraba
- 7. FP Sophates Self-organised information processing, criticality and emergence in multilevel systems
- European Commission Marko Grobelnik 17. 7. FP - NRG4CAST: Energy forecasting
- European Commission Maja Škrjanc, B. Sc.
- CIP MultilingualWeb, advancing the multilingual web European Commission Marko Grobelnik

RESEARCH PROGRAM

1. Knowledge technologies Prof. Dunja Mladenić

R & D GRANTS AND CONTRACTS

- 1. Information-communication technologies and transformation of survey research in social sciences Marko Grobelnik
- Quality of service and quality of experience measurement and control system in multimedia communications environments Marko Grobelnik
- 3. Co-authorship networks of Slovenian scholars: Theoretical analysis and visualization of user interface development
- Prof. Dunja Mladenić 4 Slovene Research Atlas
- 4. Slovene Research Atlas Prof. Dunja Mladenić
- Open communication platform for service integration Prof. Dunja Mladenić
- 6. CC CLASS: Cloud Assisted Services
- Marko Grobelnik 7. Comunication in Slovenian language
- Dr. Simon Krek 8. Topic detection and tracking
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- 10. Galit Shmueli , Indian School of Business , Hyderabad, India, 9.-13. 9. 2012
- 11. Kimberly Sellers , Georgetown University, Washington, USA, 9.-13. 9. 2012
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INDEPENDENT SCIENTIFIC COMPONENT PART OR A

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MENTORING

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LABORATORY FOR OPEN SYSTEMS AND NETWORKS E-5

The main activities of the laboratory are the R&D of next-generation networks, telecommunications technologies, components and integrated systems and information-society services and applications, especially those that ensure an efficient and pervasive life-long learning concept.

In 2012, the research group implemented the research program "Future Internet Technologies: concepts, architectures, services and socio-economic issues". Research was also carried out in the EU 7FP projects "P2P-Next" and "UNITE", the eContentplus "OpenScout" project, the "STORK 2.0" project from the CIP programme, the "SELPRAF" project from the Leonardo da Vinci programme, the "Twin Tide" project from the COST programme, and in a few national projects. The main fields of activity were technologies and services in advanced next-generation networks, security and privacy in information systems, and technology-enhanced learning. Members of the laboratory are also teaching at the undergraduate and graduate levels at the University of Ljubljana, the University of Maribor, the Jožef Stefan International Postgraduate School, and the DOBA Faculty. In 2012 they were mentors or co-mentors at one doctoral thesis, two master theses, and one diploma thesis.



Prof. Borka Jerman Blažič

Concepts, architectures, technologies and services in the future internet

Research and development of an open-source, efficient, trusted, personalized, user-centric and participatory television and media delivery system with social and collaborative connotations using the emerging Peer-to-Peer (P2P) paradigm is part of the "Next Generation Peer-to-Peer Content Delivery Platform (P2P-Next)" project. The research takes into account the existing EU legal framework and is oriented towards the development of a next-generation P2P content-delivery platform by taking into account the heterogeneous and demanding environments and the demands for a low-cost delivery of professional and user-created content. In 2012 the laboratory's contribution to the project was focused on the finalization and fine tuning of the JSI/RTV Living Lab services, a comparison of the Living Lab live video streaming with the current RTV Octoshape service, and secure access control – Enhanced Closed Swarm protocol (ECS) – in P2P systems. The laboratory has joined PlanetLab, a global research network that supports the development of new network services. The ECS protocol has been successfully tested in the PlanetLab network. The ECS protocol has been extended to work with the Peer-to-Peer Streaming Peer Protocol and submitted to IETF as an internet draft with the intention to fulfil some of the IETF Peer-to-Peer Streaming Protocol charter security requirements.

Another project in the area of the Future Internet is the "Upgrading ICT excellence by strengthening the cooperation between research teams in an enlarged Europe (UNITE)" project. The main goals of the project are the organization of researchers and PhD students exchange between EU research, academic and industrial organizations, the organization of targeted workshops, such as doctoral symposiums, across an enlarged Europe to build up synergies and support networking and collaboration, and the creation of virtual communities for the institutions involved in the research on the Future Internet.

Under the Infrastructure program in research organizations we have upgraded a video-conferencing centre. The video-conferencing centre provides the Jožef Stefan Institute with some support services that allow better communication between members of the research programs, especially in the programmes that are multi-disciplinary and the merging of multiple, geographically distributed institutions. The video-conferencing centre provides support of the Simple online communications and Advanced online communications services, which allow participants a direct view and cooperation in the distance across Europe and around the world, but their use depends on the purpose and complexity of the event. Several international video-conferencing events were organized in 2012.

Technology-enhanced learning

The laboratory has years of experience in the development of systems, services and portals for the exchange and provision of open learning material. In the "Skill-based scouting of open user-generated and communityimproved content for management education and training (**OpenScout**)" project we have, in collaboration with other partners, successfully connected different sources of open content for management education and training. The open content is available where users and institutions can easily find, access, use, and exchange open content for management education and training. Students, professionals in SMEs or large enterprises as well as teachers or course designers can easily search at learn.openscout.net for open management content that fits their specific needs. The OpenScout portal (http://learn.openscout.net) provides users with an interface to start a keywordbased search, filter search results, include competence search criteria, or add social metadata like tags, comments or ratings. Additionally, the user is presented with recommended tools for working with a selected resource. The OpenScout community enables registered users to participate in discussions and special interest groups, communicate with other community members, participate in virtual and face-to-face events, and expand their social networks.

The general aim of the Leonardo da Vinci "Self-employment with e-leaning based Practise Firms" (SELPRAF) project is to encourage people's interest in entrepreneurship through an innovative SELPRAF Training Programme for the acquisition of the four key competences and, on the other hand, to enable the inclusion of the unemployed in practice firms and to encourage self-employment. Although self-employment has been an alternative option for quite a long time, the unemployed, due to a lack of self-confidence, competence and consequently the fear of



failure, only rarely decide for this option. A more stimulating environment and stronger interest for entrepreneurship are the goals we can achieve already in the medium-term perspective with the innovative training model, based on knowledge and the transfer of practical experience. In 2012 we intensively worked on the development of interactive e-learning content, which is the basis of SELPRAF Training program. We have already chosen 100 participants for training, which will start in March 2013. With the participation in the SELPRAF training program unemployed people will gain additional knowledge and skills that they can later use in the workplace or to allow them easier access to the labour market.

The main objective of the COST project "Towards the Integration of Transectorial IT Design and Evaluation (**TwinTide**)" is to harmonize and integrate research findings and achievements with practice during the process of designing and evaluating information technologies across various sectors and disciplines. In November 2012 we co-organized in Bled an international TwinTide autumn training school TUTOREM for PhD students from the HCI field. The overarching goal of TUTOREM was to improve the participants' understanding of significant research methods commonly or increasingly used in the field of HCI. Such an enhanced understanding will enable them to select and combine the appropriate research methods for

their specific HCI projects and to contextualise them without unintended impacts on validity. The TUTOREM School was attended by 43 PhD students and 8 professors.

In 2012 we also started with two bilateral scientific cooperation projects: the first one with the Republic of Cyprus in the field of creative information spaces for problem-based learning and the second one with the Republic of Serbia within the scope of applications of workflow management technology in e-learning systems. The first results of the joint research have already been published in two international conferences. In cooperation with Lisbon University, which was carried out in the frame of the UNITE project, an analysis of business games suitable for e-learning and education was prepared. The analysis was published in an international journal.

Security, dependability and privacy in information systems

The provision of security and privacy services is crucial for the modern information society. In 2012 our activities in this field were focused on R&D in security mechanisms and services for advanced systems and networks, such as pervasive systems, P2P networks, next-generation internet systems and networks, etc., e-identity-based services, trust and reputation management, and cloud-computing security. The problems were approached in a multidisciplinary way. The first area of the research was trust and reputation management in online and social software systems. Trust and reputation of open social platforms have been systematically reviewed through General System Theory and case-study research in an article "A Holistic Approach for Designing Human-Centric Trust Systems" in the Springer journal "Systemic Practice and Action Research" with an SSCI impact factor. Systemic properties lacking in current systems have also been determined and the incorporation of social factors into design-guidelines of trust systems proposed. The organismic properties of human-centric e-commerce systems have been studied in an article "Trust as an Organismic Trait of E-Commerce Systems", published in Springer Lecture Notes, enabling a novel view of analysing trust-related design-issues, and to give notice of the possible consequences from a systemic ignorance of these issues in e-commerce systems. "Trust Transitivity and Conditional Belief Reasoning", a co-authored article in Springer Lecture Notes, proposed a novel interpretation of trust transitivity and a new mathematical model of conditional trust transitivity based on the framework of subjective logic. The second area of research was related to authorization and access control in P2P networks. An IETF internet draft was prepared and submitted for standardisation, based on previous work on an Enhanced Closed Swarm protocol developed in the P2P-Next project.

Annual Report 2012

The protocol was extended to support Peer-to-Peer Streaming IETF charter Peer protocol and its communication security additionally enhanced. In its essence the protocol merges authentication, data integrity, confidentiality, and access-control services under unified specification, extending and simplifying the current solutions like IETF Datagram TLS (DTLS).

The goal of a large "Secure identity across borders linked 2.0 (STORK 2.0)" project with 58 partners from 19 European countries is to enable e-identity-based services across borders in the fields of e-education, e-banking, public services for business, and e-health. The project that started in 2012 will demonstrate interoperable services

in real-life settings and validate common specifications, standards and building blocks, exploring scenarios to address challenging legal and governance issues (across borders, application domains and different sectors) decisively pushing the lines for the wider uptake of eID in Europe. Our initial activities included a detailed scenarios definition and the preparation of a functional specification of the common infrastructure on a European level. The laboratory will participate in the implementation and piloting of the e-education services, in particular virtual learning environment, anonymous electronic service, and job-selection service.

Electronic identity related research activities were also part of the "Cloud assisted services (CLASS)" project. The centre connects a number of Slovenian companies, universities and research institutions with an aim to develop services and products in the area of cloud computing. A result of our activities in 2012 is a security component for OpenStack that solves several



Figure 2: TUTOREM school for Ph.D. students

security problems present during the installation and running of the OpenStack platform. The solution enables the easy installation of the Object Storage (swift) and authentication and authorization (Keystone) components, and provides a secure connection between Swift and Keystone.

In the area of security-related research activities we also continued with research on security economics, where we analyse the assessment of the appropriate investment that is economically affordable and provides enough protection for the enterprise information systems. The result, i.e., an updated approach for the quantification of the necessary investment and a recommendation for a standard approach to security-information investment assessment, was published in a scientific journal "Information Processing and Management" with an SCI impact factor in the first half of the journals in informatics and management field, and in two other scientific journals.

Members of the laboratory are often invited to participate in doctoral thesis evaluation boards at foreign universities. In 2012 they were involved in the evaluation of two of these from the area of information security at the Polytechnic University of Catalonia.

Some outstanding publications in the past three years

- 1. Bojanc, R., Jerman-Blažič, B., Tekavčič, M.: Managing the investment in information security technology by use of a quantitative modeling. Inf. process. manage., 2012, vol. 48, no. 6, pp. 1031–1052
- 2. Mihajlov, M., Jerman-Blažič, B.: On designing usable and secure recognition-based graphical authentication mechanisms. Interact. comput.. [Print ed.], 2011, vol. 23, no. 6, pp. 582–593
- Dinevski, D., Poli, A., Krajnc, I., Šušteršič, O., Arh, T.: E-health integration and interoperability based on opensource information technology. Wien. klin. Wochenschr., Suppl., 2010, vol. 122, suppl. 2, pp. 3–10

Organization of conferences, congresses and meetings

- 1. Organisation of International school on HCI TUTOREM, 6.-9. 11. 2012, Bled, Slovenia
- 2. Organisation of even in frame of Bilateral cooperation, Faculty of Machinery, University of Ljubljana, Faculty of Machinery University of Niš and Laboratory for Open Systems and Networks Jožef Stefan Institute, 25. 10. 2012

INTERNATIONAL PROJECTS

- 7. FP P2P-Next: Next generation peer-to-peer content delivery platform European Commission Dr. Dušan Gabrijelčič
- 7. FP UNITE: Upgrading ICT excellence by strengthening cooperation between research teams in an enlarged Europe European Commission Prof. Borka Džonova Jerman Blažič
- eContentplus: OpenScout Skill based scouting of open user-generated and communityimproved content for management education and training European Commission Asst, Prof. Tomaž Klobučar
- STORK 2.0: Secure identity across borders Linked 2.0 European Commission Prof. Borka Džonova Jerman Blažič



- COST IC0904: Towards the integration of trans-sectorial IT design and evaluation 5 COST Office Matija Pipan, M. Sc.
- Creative multimodal information spaces for problem-based learning 6 Slovenian Research Agency Asst. Prof. Tania Arh
- Application of workflow management technology in e-learning systems 7. Slovenian Research Agency Asst. Prof. Tanja Arh

RESEARCH PROGRAM

1. Future internet technologies: concepts, architectures, services and socio-economic issues

Prof. Borka Džonova Jerman Blažič

R & D GRANTS AND CONTRACTS

- Security and trust in the new generation of P2P networks Prof. Borka Džonova Jerman Blažič Future internet collaboration platform 1
- 2. Prof. Borka Džonova Jerman Blažič
- Cloud assisted services: CC CLASS
- 3 Prof. Borka Džonova Jerman Blažič
- 4 LdV - SELPRAF: Self-employment with e-learning based practise firms Asst. Prof. Tanja Arh

NEW CONTRACT

Co-funding of future internet collaboration platform B2, d. o. o. Prof. Borka Džonova Jerman Blažič

VISITORS FROM ABROAD

- Dr. Andri Ioannou, Prof. Panayiotis Zaphiris, Christina Vasiliou, Cyprus University of Technology, CUT, Limassol, Cyprus, 17.-20. 10. 2012 1
- Prof. Miroslav Trajanović, Prof. Miodrag Manić, Prof. Miroslav Radovanović, Dr. 2 Nikola Korunović, Dušan Petković, Dr. Miloš Stojković, Asst. Prof. Dragan Mišić, Milan Zdravković, Faculty of Machinery University of Niš, Niš, Serbia, 25.-26. 10. 2012

STAFF

Researchers

- 1. Prof. Borka Džonova Jerman Blažič, Head
- Asst. Prof. Tomaž Klobučar
- Postdoctorial associates
- Dr. Tania Arh 3. Dr. Dušan Gabrijelčič 4

Postgraduates

Tanja Ažderska, B. Sc. 6. Andrej Jerman Blažič, M. Sc.

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Technical officers

Vladimir Jovanovikj, B. Sc.

Maks Mržek B Sc Matija Pipan, M. Sc

10. Svetlana Sapelova, B. Sc.

7.

8

9

11. Primož Cigoj, B. Sc., left 19.09.12 Technical and administrative staff 12. Tatjana Martun, B. Sc

> games to be used in e-learning and education", Intell. inf. manag. (Print), vol. 4, no. 6, pp. 348-356, 2012.

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1. Dejan Dinevski, Tanja Arh, "Web 2.0 technologies for e-learning", In: *Global e-learning*, Ana Landeta Etxeberria, ed., [Madrid], CEF, [2012], pp. 175-184.

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DEPARTMENT OF COMMUNICATION E-6 **SYSTEMS**

The core activities of the Department of Communication Systems comprise the research, development and design of next-generation telecommunication networks, technologies and services; wireless communication, embedded and sensor systems; and new procedures and algorithms for parallel and distributed computing. Within these activities our research work includes the development of the methods and software tools for modelling, simulation, analysis and synthesis of communication systems, computer simulations supporting biomedical procedures and specialised equipment and procedures for advanced bio-signal processing and interpretation.

Research and development activities at the department are carried out in the framework of the Communication Technology Laboratory (CTL), the Parallel and Distributed Systems Laboratory (PDSL) and the Networked Embedded Systems Laboratory (NESL). The research work of the three laboratories is complementary, which is reflected in the joint applied projects.

In 2012 the research activities within the Communication Technology Laboratory were concentrated on different challenges associated with the access-segment technologies enabling the end-users to access new multimedia Asst. Prof. Mihael Mohorčič services and applications. As part of the multi-year telecommunication-systems research programme the emphasis was on research in the areas of: radio propagation, access architectures for heterogeneous wireless networks,

management of radio and network resources and cognitive communications. The investigation of the radio-signal propagation was focused on two main topics. The first topic concerns the research of the radio-signal propagation in special environments, such as long road and railway tunnels, used for emergency situations. The emphasis was on the radio-signal propagation in typical frequency bands for voice communication systems (400 MHz), high-speed data communication systems (2.4 GHz and 3.5 GHz) and low-data-rate wireless sensor networks (868 MHz and 2.4 GHz). The second topic, researched in cooperation with Mobitel, d. d. and Telekom Slovenije, d. d., concerns the development, implementation and testing of the software modules for the radiowave-propagation modelling in mobilecommunications systems for rural and urban environments including statistical channel models as well channel models based on ray tracing and its integration into the open-source geographic information system (GIS).

A research into efficient acceleration techniques for radio ray-tracing using massively parallel hardware has been started. An optimization method applicable to a wider set of problems solved by SIMD processors was proposed.

In collaboration with Telekom Slovenije we conducted a computer simulation-based performance evaluation of the introduction of new services in their network. For this purpose we developed a comprehensive simulation model of the fixed network of Telekom Slovenije. We also analysed typical patterns of network alarms and developed an alarm mining and prediction tool. We continued the investigation of advanced concepts and technologies for a capacity increase of wireless meshed networks using network coding techniques. In particular, we focused on the development of advanced network coding algorithms and their adapted routing procedures. In order to support the performance evaluation of arbitrary network coding algorithms on predetermined or randomly generated topologies of wireless meshed networks, we designed and built a simulation model, which allows the performance evaluation of network coding algorithms and routing procedures.

In collaboration with European partners we started the ABSOLUTE "Aerial Base Stations with Opportunistic Links For Unexpected & Temporary Events" - project, the main objective of which is to design and validate an innovative rapidly deployable future network architecture which is resilient





Figure 1: We published at InTech two book chapters, one in Salim N. Kazi (Ed.). Heat transfer phenomena and applications. InTech, 2012, ISBN 978-953-51-0815-3, and one in Jesus Hamilton Ortiz (Ed.). Telecommunications Networks - Current Status and Future Trends. InTech, 2012, ISBN 978-953-51-0341-7.

- For integration in the open-source geographic information systems GRASS, we developed and implemented a software module for radio-wave-propagation modelling in mobile communication systems based on ray tracing.
- We developed and implemented a highperformance software tool TopoSWiM for the topology design and accessibility provision in large-scale wireless mesh networks.
- We designed and developed new hardware and software modules and implemented new features for the VESNA platform.



Figure 2: Comparison of satellite-signal attenuation with rainfall measurements

and capable of providing broadband multi-service, secure and dependable connectivity for large coverage areas affected by large-scale unexpected events (or disasters) leading to the partial or complete unavailability of the terrestrial communication infrastructure or for temporary events leading to the demand for very high throughput and augmented network capacity.

In 2012 we were actively participating in several COST actions. In COST Action IC0802 "Propagation tools and data for integrated Telecom, Navigation and Earth Observation systems" we were active in two working groups. In WG2 we designed new algorithms for satellite signal processing, in WG3 we worked on new channel models for free-space optical links. In the COST Action IC0902 "Cognitive Radio and Networking for Cooperative Coexistence of Heterogeneous Wireless Networks" we integrated two low-cost VESNA-based spectrum sensing nodes in a heterogeneous spectrum sensing platform built by the University of Ss. Cyril and Methodius in Skopje, and evaluated the performance of different sensing agents. In the COST Action

IC1101 "Optical Wireless Communications – An Emerging Technology" we investigated in cooperation with TU Graz the influence of weather conditions on the performance of a hybrid RF-FSO network and published the research results in the journal IET Communications. We also joined a new COST Action IC1104 "Random Network Coding and Designs over GF(q)", in which we are developing practical network coding procedures and evaluating them in a purpose-built simulation model.

In the PECS project SatProSi we developed for European Space Agency our own Beacon Receiver for the EU-TELSAT HotBird 6 signal.

- For the needs of different projects we started with the deployment of a sensor-network-based testbed LOG-a-TEC, supporting experimental research in radio and networking areas and in the Internet of Things applications.
- In the frame of the EU 7FP CREW project and the FIRE initiative the LOG-a-TEC testbed is used as a real-life outdoor experimental environment for cognitive radio and cognitive networking research.

In the area of cognitive communications we continued research in the radio and access segments and contributed to the WUN-CogCom and 7FP CREW projects. In 2012 our research in this area was focused on stand-alone and collaborative spectrum sensing in licensed and unlicensed frequency bands and on building radio environmental maps.

In cooperation with the Department of Low and Medium Energy Physics (F2) we continued research activities started in previous years that were focused primarily on efficient signal-processing algorithms in high-count-rate gamma-ray spectrometry.

In the **Parallel and Distributed Systems Laboratory**, we successfully continued interdisciplinary research work in the framework of an enhanced program group, and we were joined by colleagues from the University of

Ljubljana, the Machine Vision Laboratory from the Faculty of Electrical Engineering and the Laboratory for Algorithms and Data Structures from the Faculty of Computer and Information Science. We were heavily involved in research within the research program Parallel and Distributed Computing and also in other research projects. Our cooperating researchers also come from industry (Turboinstitut d.d. and Xlab d.o.o.) and from the medical sphere (the University Clinical Center Ljubljana).



Figure 3: Sensor Node Core module of the VESNA platform

We investigated computer algorithms for efficient implementation on parallel and distributed computers, testing them on a research cluster computer, which runs at our department, and on a cloud recently installed in cooperation with the Faculty of Computer and Information Science of the Ljubljana University and Turboinstitut d.d. In addition to demanding computations, we also paid attention to distributed large data storage. We continued investigations in the field of wireless sensor networks based on the theory of parallel and distributed computing and communication.

We developed new parallel numerical algorithms, e.g., meshless methods, which are local and, hence, efficiently executable on parallel computers. With these methods, one can simulate physical phenomena, e.g., heat and fluid flows, PN junctions and molecular dynamics in realistic conditions. We developed software for simulating biological systems, e.g., lipid membranes and biomedical procedures, such as post-surgical cryotherapy and RF, and cryo-ablation of the heart. We parallelized multi-criterion optimizations and began to investigate how to efficiently integrate measurement results, simulation results and optimization methods, which will enable us to predict biological parameters that are hard to measure in a non-invasive manner. We developed a new methodology for synthesising the standard ECG from a small number of differential measurements. We investigated possible options for an analysis of large signal sets with the human auditory system (sonification). We investigated possible options for the detection of respiratory sinus arrhythmia (RSA) in the ST interval. We developed a new method for measuring the variability of the ST interval with a sub-millisecond resolution. Together with neurologists from the University Clinical Center Ljubljana, we continued equipment upgrading and measurements for the NeuroECG.

In the field of formal methods for discrete systems modelling and development, we investigated the isomorphicity-test synthesis for the deterministic final-state machines, also for the needs of distributed testing, proposing improved algorithms and stronger state-recognition principles.

In 2012 the Networked Embedded Systems Laboratory mainly focused on research and development in the areas of the Internet of Things and cognitive communications. The emphasis was on the vertical integration of different wireless sensor and communication network technologies with semantic technologies in the support of the autonomous search and composition of sensors and sensor data, as well as on the development of new applications using various machine-learning and decision-making algorithms. These activities were mainly conducted within the basic research project "Advanced procedures for interactive composition of sensor networks" and the EU FP7 Network of Excellence PlanetData.



Figure 4: Optimal gateway locations, estimated by TopoSWiM, a software tool for the topology design of large-scale wireless mesh networks.

The modular and fully flexible wireless sensor networks platform VESNA, developed as the core building block for several research and applied projects, has been complemented with a set of new modules and features, including radio spectrum sensing in the UHF and ISM frequency bands within the EU FP7 CREW project, a suite of motion, location, presence and ambient sensors within the national competence centre KC OpComm, a framework for the semantic description of sensor node functionalities and status, wired and wireless gateway capabilities for internet

connectivity or interaction with other devices, etc. A variety of supported features, protocols and technologies, together with the arbitrary combination of developed hardware and software modules, make the VESNA platform well suited for the implementation of experimental research sensor networks infrastructure, the deployment of pilot applications, the validation of usage scenarios and the development of end-user solutions.

In collaboration with the Municipality of Logatec and Komunalno podjetje Logatec we deployed a large-scale outdoor wireless sensor network, which represents the initial version of our LOG-a-TEC experimental testbed and thereby the baseline for different basic and applied projects. The testbed is based on the VESNA platform and equipped with a set of sensors and communication interfaces, as required by a given project. The sensor nodes' firmware

management, the execution of experiments and the gathering of sensor measurements data is performed via a web application running on one of our servers. In the current setup built for the FP7 CREW project the LOG-a-TEC testbed consists of more than 50 nodes in two clusters and allows the execution of experimentally-driven research in the areas of spectrum sensing in licensed and unlicensed frequency bands, cognitive radio and cognitive networking. As a part of the CREW testbeds federation this part of LOG-a-TEC also represents one of the FIRE facilities, i.e., the only one supporting the investigation of horizontal and vertical radio-spectrum-sharing methods in a real-life out-

door environment and being particularly well suited for experiments in TV white spaces. The LOG-a-TEC testbed has been complemented with another location at JSI, where VESNA platforms are equipped with Contiki OS and intended for experimentation with cognitive networking on MAC and higher layers using the ProtoStack tool for remote composition, reconfiguration and reprogramming of the CRime protocol stack.

Our research work in the frame of the national competence centre KC OpComm, aiming at the development of an open communication platform for the development of new types of services and applications for the Future Internet, is concentrated on the provision of data and context information from sensor networks to management services and applications. To this end,

- We have compared the calculation complexities of different meshless methods for solving a diffusion equation and concluded that strong formulated approaches are computationally more efficient than weak formulations.
- We have developed a prototype wireless electrode of bio-potentials from the body surface for the concurrent measurements of an ECG and the respiration rate.



Figure 5:Average temperatures of all patients during cooling treatment in Group A with the gel-pack (left) and Group B with the cTreatment® (right). Abbreviations: ICN - intercondylar notch, SC - subcutaneous, SKskin (12 – anterior, 3 – medial, 6 – posterior, 9 - lateral), BA - bandage.



Figure 6: Results of a numerical simulation of binary material solidification (Sn-10%Pb). Concentration and velocity fields are presented at the moment when instabilities appear (left), and in the steady state (right). In the steady state the mesosegretaes, which are still not understood, are visible (areas filled with high concentration).

- We synthesised, with a high reliability, a standard 12-lead ECG from three bipolar wireless electrodes.
- We improved a simulation model for the performance evaluation of network-coding techniques.

we continued developing different VESNA platform modules, investigating procedures for the preprocessing of data and metadata, and developing the required communication protocols and interfaces for the platform. Related to these activities we developed sensoric support for an asset-management application and remote monitoring of the photovoltaic power plant at Telekom Slovenije.

In the area of remote monitoring we continued the work in the EU FP7 project BalkanGEONet concerned with the inclusion of all Balkan countries into GEO. In the area of wireless sensor networks we also started with two new FP7 projects. In the Absolute project our role is to integrate a VESNA-based wireless sensor network in the emergency communications network architecture. The aim is to provide easily deployable sensor network for in-situ fixed or participatory monitoring of post-disaster parameters as well as for the spectrum sensing needed to support the ad-hoc establishment of the Absolute communication system without causing harmful interference to coexisting communication systems. In the CITI-SENSE project, which is concerned with the establishment of sensor-based Citizens' Observatory Community for improving the quality of life in cities, our focus is mainly on providing the VESNA-based solution for air-quality monitoring. As part of this we are developing modules with gas, particle matter and other ambient related sensors, which will be used for indoor and outdoor environment monitoring.

The Networked Embedded Systems Laboratory and its research and development activities also take part in the SensorLab group, which was established by the Department of Communication Systems and the Laboratory of Artificial Intelligence.

Some outstanding publications in the past year

- 1. Nadeem, F., Leitgeb, E., Kandus, G., Javornik, T.: Comparing the cloud effects on hybrid network using optical wireless and GHz links. IET communications. 2012, vol. 6, no. 5, pp. 492–498
- 2. Hrovat, A., Kandus, G., Javornik, T.: Path loss analyses in tunnels and underground corridors. Int. j. commun., 2012, vol. 6, no. 3, pp. 136–144
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- Trobec, R., Rashkovska, A., Avbelj, V.: Two proximal skin electrodes a respiration rate body sensor. Sensors. http://www.mdpi.com/1424-8220/12/10/13813
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Organization of conferences, congresses and meetings

- 1. Workshop on collecting, processing and the application of environmental and spatial data in Slovenia", Reactor Centre Podgorica, Podgorica, Slovenia, 12. 2. 2012
- 2. CREW plenary meeting, Ljubljana, Logatec, 18.-21. 6. 2012

Awards and appointments

- 1. Tomaž Šolc: Award for the best paper for article "Spectrum Sensing for Cognitive Wireless Applications Inside Aircraft Cabins", 31st 2012 IEEE/AIAA Digital Avionics Systems Conference, Williamsburg, Virginia, USA, 14.–18. 10. 2012
- 2. Urban Kuhar: First place on the student competition for article "The design of a low-cost beacon receiver based on software defined radio", 21st International Electrotechnical and Computer Science Conference, Portorož, 18.9. 2012

Patent granted

1. Roman Novak, Matjaž Vencelj, Method for quantum distribution of the short-range key, SI23596 (A), Urad RS za intelektualno lastnino, 29.6.2012

INTERNATIONAL PROJECTS

- 7FP PlanetData 1. European Commission
- Asst. Prof. Mihael Mohorčič
- 7FP BalkanGEONet: Balkan GEO network-towards inclusion of Balkan countries into 2. global Earth observation initiatives
- European Commission Asst. Prof. Mihael Mohorčič
- 7FP CREW: Cognitive radio experimentation world 3. European Commission
- Asst. Prof. Mihael Mohorčič
- 7FP ABSOLUTE: Aerial base stations with opportunistic links for unexpected and 4. temporary events
 - European Commission Asst. Prof. Mihael Mohorčič
- 7FP CITI-SENSE: Development of sensor-based citizens' observatory community for 5 improving quality of life in cities European Commission
 - Asst. Prof. Mihael Mohorčič
- ESA PECS: Processing of satellite signals in Ka/Q-frequency band 6. ESA/ESTEC
 - Prof. Gorazd Kandus
- COST IC1004: Cooperative radio communications for green smart environments 7. COST Office
- Asst. Prof. Tomaž Javornik
- 8. COST IC1101: Optical wireless communications - an emerging technology COST Office
- Prof. Gorazd Kandus COST IC0906, WiNeMO: Wireless networking for moving objects COST Office
- Miha Smolnikar, B. Sc.
- 10. COST IC0902: Cognitive radio and networking for cooperative coexistence of heterogeneous wireless networks COST Office
 - Asst. Prof. Mihael Mohorčič
- 11. COST IC0805: Open European network for high performance computing on complex environments COST Office
 - Prof. Roman Trobec
- 12. COST IC0802: Propagation tools and data for integrated telecommunication, navigation and Earth observation systems COST Office
- Prof Gorazd Kandus
- 13. HiPEAC: European Network of Excellence on high performance and embedded architecture and compilation

VISITORS FROM ABROAD

- Prof. dr. Veljko Milutinović, Faculty of Electrotechnics, Belgrade, Serbia, 25 May 2012 1. Prof. dr. Oskar Mencer, Maxeler Technologies and Imperial College London, London, 2
- Great Britain, 25 May 2012
- Dr. Goran Dimić, Institute "Mihailo Pupin", Belgrade, Serbia, 25 May 2012 3 Adnan Bekan, Faculty of Electrical Engineering Tuzla, Tuzla, Bosnia, 15 July to 28 4.
- September 2012 5
- Prof. Ingrid Moerman, Interdisciplinary Institute for Broadband Technology, Ghent-Ledeberg, Belgium, 18-21 June 2012
- Prof. dr. Luiz DaSilva, University of Dublin, Dublin, Ireland, 18-21 June 2012 6.
- Peter Van Wesemael, IMEC, Leuven, Belgium, 18-21 June 2012
- Jan Hauer, Technische Universität Berlin, Berlin, Germany, 18-21 June 2012 8
- Mikołaj Chwalisz, Technische Universität Berlin, Berlin, Germany, 18-21 June 2012 9.
- 10. Alejandro Sanchez, Thales Communications France, Neuilly-sur-Seine Cedex, France, 18-21 June 2012
- 11. Dr. Stefan Bouckaert, Interdisciplinary Institute for Broadband Technology, Ghent-Ledeberg, Belgium, 18-21 June 2012
- 12. Danny Finn, University of Dublin, Dublin, Ireland, 18-21 June 2012

Ghent University Prof Roman Trobec

- 14. VHP NoE: Virtual physiological human network of excellence University College London Prof. Roman Trobec
- 15. Cellular and finite automata for structure recognition Slovenian Research Agency
- Prof. Roman Trobec 16. Advanced technologies for next generations of mobile broadband communication
 - systems Slovenian Research Agency
 - Asst. Prof. Tomaž Javornik
- Optimization of energy consumption in distributed computing systems Slovenian Research Agency Prof. Roman Trobec

RESEARCH PROGRAMS

- Telecommunication systems Prof. Gorazd Kandus
- Parallel and distributed systems 2 Prof. Roman Trobec

R & D GRANTS AND CONTRACTS

- 1. Advanced procedures for interactive composition of sensor networks Asst. Prof. Mihael Mohorčič
- Learning, analysis, and detection of motion in the framework of a hierarchical 2 compositional visual architecture Prof. Roman Trobec
- Open communication platform for service integration: CC OPCOMM 3 Asst. Prof. Mihael Mohorčič
- 4 Cloud Assisted Services: CC CLASS Prof Roman Trobec

NEW CONTRACT

- 1. Parallelization of the pathloss modules for GRASS-RaPlaT and implementation of new pathloss modules for urban environment Telekom Slovenije, d. d. Asst. Prof. Tomaž Javornik
- 13. Andre Puschmann, Ilmenau University of Technology, Ilmaneu, Germany, 18-21 June 2012
- 14. Christoph Heller, EADS, Munchen, Germany, 18-21 June 2012
- 15 Dr. Vaclav Kvičera, Czech Metrology Institute, Brno, Czech Republic, 24-26 September 2012 16. Dr. Ondrej Fišer, Institute of Atmospheric Physics, Prague, Czech Republic, 24-26
- September 2012
- Prof. Fary Zabih Ghassemlooy, Northumbria University, Newcastle, Great Britain, 24-26 17. September 2012
- 18. Prof. Faruk Özek, Faculty of Engineering, Ankara University, Ankara, Turkey, 24-26 September 2012
- 19. Prof. Erich Leitgeb, Institute of Broadband Communications, Graz University of Technology, Graz, Austria, 24-26 September 2012
- 20. Maja Ilić Delibašić, Faculty of Electrical Engineering, Podgorica, University of Montenegro, Montenegro, 10-12 December 2012
- 21 Dr. Venceslav Kafedziski, Faculty of Electrical Engineering and Information Technologies, Skopje, Macedonia., 1 April – 31 August 2012
- 22. Prof. Karolj Skala, Institute Ruđer Bošković, Zagreb, Croatia, 14-17 November 2012

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- 14. Dr. Gregor Kosec
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- 16. Dr. Andrej Vilhar
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- 18. Carolina Fortuna, B. Sc.
- 19. Erik Pertovt, B. Sc.
- 20. Marko Pesko**
- 21. Aleksandra Rashkovska, B. Sc.

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- Carolina Fortuna, Marko Grobelnik, "From sensors to real-time analytics", *Elektrotehniški vestnik*, vol. 79, no. 5, pp. 273-277, 2012.
- 3. Julia Genova, Janez Ivan Pavlič, "Realization of Marin Mitov idea for the stroboscopic illumination used in optical microscopy", *Bulg. J. Phys.*, vol. 39, no. 1, pp. 65-71, 2012.
- 4. Andrej Hrovat, Gorazd Kandus, Tomaž Javornik, "Path loss analyses in tunnels and underground corridors", *Int. j. commun.*, vol. 6, no. 3, pp. 136-144, 2012.
- 5. Siraj-ul- Islam, Božidar Šarler, Robert Vertnik, Gregor Kosec, "Radial basis function collocation method for the numerical solution of the two-dimensional transient nonlinear coupled Burgers' equations", *Appl. math. model.*, vol. 36, issue 3, pp. 1148-1160, 2012.
- 6. Monika Kapus-Kolar, "New state-recognition patterns for conformance testing of finite state machine implementations", *Comput. stand. interfaces*, vol. 34, no. 4, pp. 390-395, 2012.
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- 9. Gregor Kosec, "Simulation of multiphase thermo-fluid phenomena by a local meshless numerical approach", *Informatica (Ljublj.)*, vol. 36, no.2, pp. 227-228, 2012.
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22. Miha Smolnikar, B. Sc.
23. Tomaž Šolc, B. Sc.
24. Matevž Vučnik, B. Sc. **Technical and administrative staff**25. Polona Anžur, B. Sc.
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MENTORING

- 1. Robert Blatnik, *Influence of the voice quality in telephony on the automated speaker recognition:* master's thesis, Ljubljana, 2012 (mentor Gorazd Kandus; co-mentor Tomaž Šef).
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COMPUTER SYSTEMS DEPARTMENT E-7

The department is concerned primarily with the design automation of computing structures and systems. Within this broad area, we are concentrating on the meta-heuristic approach to engineering design and logistics problems as well as system design and test. As an integral part of our research activity, members of the department have close contacts and collaborations with scientists worldwide, through academic links and industrial contacts, thus enabling us to keep at the forefront of this rapidly developing field.

In the field of computer structures we are concentrating on the design of FPGA-based reconfigurable systems for selected target applications.

In the area of hardware/software co-design we collaborate with the Faculty of Electrical Engineering and Computer Science, University of Maribor. Within the application project we are developing a hardware accelerator for the compression of LIDAR data. In the past year, hardware predictors of the point coordinates and other attributes of LIDAR data were developed. The predictors of the point coordinates consist of two methods: linear prediction Head: using last coordinate changes, and the search for the closest coordinate change among the most recent coordinate Prof. Franc Novak changes. The applied method is dynamically selected based on the resemblance of the current search result. A pipelined hardware divider, required for linear prediction, was also developed. An adjustable pipeline depth enabled us to select the most suitable divider with respect to the dividers' latency, the usage of the hardware resources, and the clock period. The coordinate prediction and the prediction of other LIDAR data attributes are used in the predic-

tion compression of the LIDAR data. Additionally, a variable length encoder was developed, and the arithmetic coder was improved by using the barrel shifter structure, which resulted in up to 8-times higher data throughput. Modules were developed in the VHDL language and verified in the Cadence simulation environment. Individual modules were synthesized and tested on the Xilinx XUPV5 prototype board.

We developed a portable, pocket-sized, wireless, kitchen scale that informs diabetic patients about the carbohydrate content of foods in realtime.

The application of SRAM-based field-programmable gate arrays (FPGAs) in mission-critical systems requires error mitigation and recovery techniques to protect them from the errors caused by high-energy radiation, also known as single-event upsets (SEUs).

We developed a SEU-recovery mechanism with a smaller hardware overhead than the existing solutions. According to the required levels of reliability, the mechanism can be employed in different self-recoverable architectures.

The efficiency of the proposed approach was evaluated with a specially developed fault-emulation environment. In contrast to conventional statistical methods based on radiation techniques, the developed fault emulation enables the user to inject faults at selected locations of the configuration memory. Then, individual parts of the recovery infrastructure can be analysed. In this way, modifications and possible improvements to the recovery infrastructure can be easily evaluated.

The resulting estimated reliability of our error-recovery mechanism is superior to the other reported solutions. It supports the Xilinx Virtex 4 and Virtex 5 FPGA families, and it can be easily extended to include Virtex 6 devices. The same recovery principle can also be applied to the FPGA devices of other manufacturers.



An important part of our research activities is related to the development of metaheuristic optimization methods and their applications. We have developed the continuous differential antstigmergy algorithm (CDASA) and evaluated it on real-world optimization problems.

Within an industrial project for ETA Cerkno d.o.o. we upgraded the application for product planning and management. The company produces components for domestic appliances, including cooking plates, thermostats, and heating elements. There are many different models due to the various demands of other companies that need cooking plates for their own cooking appliances. So the production must be scheduled very carefully to fulfil all the demands (quantities and deadlines), to maintain the specified amount of different models in stock, to optimally





occupy their workers, and to efficiently use all the production lines. The upgraded application introduces a multiobjective approach to production scheduling.

Within a project with Gorenje, d. d., Velenje, we were developing a program tool for the simulation and optimization of temperatures inside a refrigerator. For the optimum working of a refrigerator the desired temperature is

Research of "On-line testing and recovery of FPGA-based systems" was published in the journal IEEE Transactions on Nuclear Science. sustained with the lowest possible power consumption. With a simulator that allows the simulation of temperatures inside the refrigerator during different modes of regulation, we replace the part of the measurements that are time consuming due to the slow thermal processes. The integrated optimization algorithm automatically finds the optimal regulation of a refrigerator. The

developed tools allow the substitution of a several-day observation of a refrigerator with a several-second simulation. This substitutes a large set of measurements and lowers the development costs.

In the area of machine vision we finished a project for the company Tesnila GK d.o.o. where the aim was to develop a quality-control machine-vision solution for various rubber parts produced by the company. The procedure includes a fast dimensional inspection of each rubber part, resulting in the replacement of the slow manual inspection.

In the area of computer vision we continued with the development of an automated cell-counting procedure based on an artificial neural network optimization of image processing to be used in an electroporation treatment. A new version of the software platform was implemented that helps researchers to quickly obtain the number of biological cells in a large number of image series by manually counting cells in only a few images. The tested accuracy is over 90%, which is comparable to user manual counting, especially when taking into account inter-person error, which can be up to 10%.

In collaboration with the Faculty of Health Studies, University of Ljubljana, we continued our work on the Wartenberg pendulum test, where the time dependence of a knee angle is tracked and then compared to a damped oscillation curve. The parameters of this curve are used to determine the viscosity of a knee's synovial fluid and to detect anomalies. Several groups of people were tested, belonging to different age populations, some of them being affected by diabetes. The developed procedure was used to obtain the results within two diploma works at the Faculty of Health Studies.

In collaboration with the Paediatric Clinic, the University Medical Centre Ljubljana, and the Biotechnical Faculty,



Figure 2: Organization of the fifth biennial international conference on bioinspired optimization methods and their applications.

University of Ljubljana, we carried out a clinical study on the usability of "Open Platform for Clinical Nutrition" (OPEN; http://opkp.si) for research purposes. In the study, 150 participating pregnant and lactating women tracked four-day food diaries with the help of clinical dieticians. We have analysed the correctness of the calculation of the energy and nutrition logs for all the nutrients that are vital for pregnant and lactating women. The calculated values will be compared with the analytical values. The results of the study are crucial for the continuation of work in this area.

In cooperation with the Slovenian Society for Clinical Nutrition, we carried out a national survey "Assessment of nutritional status of patients and the elderly in Slovenia". For this purpose we developed a mobile application that integrates different tools for the dietary screening of malnourished patients of different ages and health conditions. The mobile application is an upgrade of OPEN and allows the easy transition to the web application, where patients facing malnutrition can find more information and tools for planning an appropriate diet. By using tablets and mobile applications, selected clinical dieticians carried out dietary screening at the Institute of

Oncology Ljubljana; Clinical Gastroenterology Department of the Internal Clinic of the University Medical Centre Ljubljana; and the Hospital Dr Petra Držaja, Ljubljana.

In collaboration with the Paediatric Clinic, University Medical Centre Ljubljana and the Faculty of Social Sciences of the University of Ljubljana, we carried out a national survey "Water wins" (http://vodazmaga.si/), which aims to encourage children aged 11 to 14 to drink fewer sugary drinks and replace sugary drinks with water and other unsweetened beverages. To OPEN, we included a photo food questionnaire, which was completed by 300 primary-school children. The questionnaire was upgraded with a module for a statistical analysis of the responses and thus provided an added value to OPEN for the purposes of many other studies in this field.

In 2011 we finished the targeted research project "Slovenian food table - plant foods", the coordination of which was conducted at the Biotechnical Faculty, University of Ljubljana. In collaboration with the Department of Low and Medium Energy Physics, we developed an electronic food composition of plant foods and harmonized it with the pan-European distributed database EuroFIR.

We developed a portable, pocket-size, wireless kitchen scale that informs diabetic patients about the carbohydrate content of foods in real-time. The scale is wirelessly connected with a mobile phone, a tablet or a computer that has internet access and runs OPEN. This embedded system may also be used by other patients with special nutritional needs, as well as by researchers.

Within the European project EuroFIR NEXUS we have participated in the program modelling, implementation and testing of an information platform that integrates information systems of 50 EuroFIR Member States. We supervised the development of a food browser, FoodExplorer, and a recipe-calculation tool, FoodBasket. Also, we have developed an advanced heuristic algorithm for the optimal searching of foods similarly categorized by LanguaL, which enables the efficient exchange of data from different electronic food-composition databases.

To support a national study on malnutrition in Slovenia, we developed a mobile application that integrates different tools for the dietary screening of malnourished patients of different ages and with various health conditions.

Under the supervision of EuroFIR AISBL, we run an international project "Updated food composition database for nutrient intake", which is aimed at the creation of a European food-composition database for the European Food Safety Authority (EFSA) in an appropriate electronic format. The data were categorized according to the standard FoodEx2 that allows the harmonization of EU food-consumption data.

In 2012 we began a bilateral cooperation with the Portuguese national institute Instituto Nacional de Saúde Dr. Ricardo Jorge in Lisbon. We cooperate within the Portuguese project "Exploring the Effects of Toxic Mixtures of mycotoxins and infant food and potential health impact", in which OPEN has been upgraded with a user interface in Portuguese, the Portuguese food composition database and tools for monitoring the toxic ingredients of baby food and beverages.

In cooperation with Department of Intelligent Systems we organized the BIOMA 2012 conference (Bioinspired Optimization Methods and their Applications). The fifth biennial conference included presentations and discussions on the newest theoretical and practical results on nature-inspired optimization methods and their applications. The conference presentations are included in the conference proceedings.

In cooperation with the Department of Intelligent Systems and the Laboratories for Computer Architecture and Languages and Programming Methodologies from the Faculty of Electrical Engineering and Computer Science, University of Maribor, we organized, for the seventh consecutive year, the workshops on "Nature-inspired algorithms" about stochastic optimization techniques.

Some outstanding publications in the past three years

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- 3. Legat, U., Biasizzo, A., Novak, F.: SEU recovery mechanism for SRAM-based FPGAs. IEEE trans. nucl. sci., 2012, vol. 59, no. 5, pp. 2562–2571
- 4. Pavlin, M., Novak, F.: A Wireless Interface for Replacing the Cables in Bridge-Sensor Applications. Sensors, 2012, vol. 12, no. 8, pp. 10014-10033
- Papa, G., Vukašinović, V., Korošec, P.: Guided restarting local search for production planning. Eng. Appl. Artif. Intell., 2012, vol. 25, no. 2, pp. 242–253

Organization of Conferences, Congresses and Meetings.

- The 5th International Conference on Bioinspired Optimization Methods and their Applications, BIOMA 2012, Bohinj, 24–25 May 2012
- 2. AVN, The 20th workhoop Nature-Inspired Algorithms, 20 September 2012, Šmarna gora, Slovenia

INTERNATIONAL PROJECTS

 7. FP - EuroFIR-Nexus: The EuroFIR Food Platform: Further integration, refinement and exploitation of for its long-term self-sustainability European Commission

Asst. Prof. Barbara Koroušić Seljak

- EFSA: Updated food composition database for nutrient intake European Food Safety Authority - EFSA Asst. Prof. Barbara Koroušić Seljak
- COST IC1204: Trustworthy manufacturing and utilization of secure devices COST Office Prof. Franc. Novak
- HIPEAC: European Network of Excellence on high performance and embedded architecture and compilation Ghent University Prof. Franc Novak



RESEARCH PROGRAM

1. Computer Structures and Systems Prof. Stanislav Kovačič

R & D GRANTS AND CONTRACTS

- 1. Processing of massive geometric LIDAR data Prof. Franc Novak
- 2. Food composition tables plant-derived foods Asst. Prof. Barbara Koroušić Seljak

VISITOR FROM ABROAD

 Dr. Eva Balsa-Canto, researcher from Bioprocess Engineering Group, IIM-CSIS Spanish National Council for Scientific Research, Vigo, Spain, 28–31 May 2013

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 eDietitian: Mobile diet guide Asst. Prof. Barbara Koroušić Seljak

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11. Dr. Uroš Legat, left 01.06.12

ORIGINAL SCIENTIFIC ARTICLE

- Petr Gregor, Riste Škrekovski, Vida Vukašinović, "Queue layouts of hypercubes", *SIAM j. discrete math.*, vol. 26, no. 1, pp. 77-88, 2012.
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- 11. Katerina Taškova, Jurij Šilc, Nataša Atanasova, Sašo Džeroski, "Parameter estimation in a nonlinear dynamic model of an aquatic ecosystem with meta-heuristic optimization", *Ecol. model.*, vol. 226, no. 1, pp. 36-61, 2012.

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- 13. Katerina Taškova, Jurij Šilc, Peter Korošec, "Exploring the parameter space of a search algorithm", In: *Bioinspired optimization methods and their applications: proceedings of the Fifth International Conference on Bioinspired Optimization Methods and their Applications - BIOMA 2012,* 24-25 May 2012, Bohinj, Slovenia, Bogdan Filipič, ed., Jurij Šilc, ed., Ljubljana, Jožef Stefan Institute, 2012, pp. 151-162.
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INDEPENDENT SCIENTIFIC COMPONENT PART OR A

CHAPTER IN A MONOGRAPH

 Asta Gregorič, Boris Zmazek, Sašo Džeroski, Drago Torkar, Janja Vaupotič, "Radon as an earthquake precursor - methods for detecting anomalies", In: *Earthquake research and analysis: statistical studies, observations and planning*, Sebastiano D'Amico, ed., Rijeka, InTech, cop. 2011, pp. 179-196.

MENTORING

- 1. Uroš Legat, *On-line testing and recovery of FPGA-based systems:* doctoral dissertation, Ljubljana, 2012 (mentor Franc Novak).
- Katerina Tashkova, Parameter identification in nonlinear dynamic systems with meta-heuristic approaches: doctoral dissertation, Ljubljana, 2012 (mentor Sašo Džeroski; co-mentor Jurij Šilc).

DEPARTMENT OF KNOWLEDGE **TECHNOLOGIES** E-8

The Department of Knowledge Technologies performs research in advanced information technologies aimed at acquiring, storing and managing knowledge to be used in the development of knowledge-based applications. Established areas include intelligent data analysis (machine learning, data mining, and knowledge discovery in databases), semantic data mining and the semantic web, language technologies and computational linguistics, decision support and knowledge management. Apart from research in knowledge technologies, we are also developing applications in environmental sciences and ecology, medicine and health care, biomedicine and bioinformatics, economy and marketing.

In 2012 we were involved in eight national and thirteen European projects, most of them funded in the seventh framework program (FP7). In terms of our collaboration in EU projects, we were the most successful program group in Slovenia.

In the area of intelligent data analysis and data mining we have developed several new methods and used Head: them in a number of application areas. We developed a new approach for creating and implementing data-mining **Prof. Nada Lavrač** workflows, upgrading the service-oriented knowledge-discovery platform Orange4WS, also developing a new workflow platform called ClowdFlows. In Orange4WS we also developed and implemented a novel SDM-Toolkit used

for semantic subgroup discovery; a new triplet extraction methodology from text, used for signaling network construction in the modeling of plant defense response; and the SegMine methodology, which together with the BioMine system for the detection of new links between genes, allows for semantic gene expression analysis by using bio-ontologies as background knowledge.

We developed a new system for bisociative knowledge discovery called CrossBee, used for discovering new connections between different medical domains. We developed a new methodology for mining document-enriched heterogeneous information networks and a new approach to equation discovery, enabling the learning of process-based models of dynamic systems

from data and domain knowledge, which can use different criteria and methods for parameter optimization. We developed new methods for learning rule ensembles for multi-target regression and new methods for multi-label classification and conducted a large-scale empirical comparison of existing ones. We used the newly developed methods in a number of environmental problems, including the hierarchical classification of diatoms from images, modeling the dynamics of aquatic ecosystems, and modeling gene flow between conventional and genetically modified crops.

We have successfully concluded our work on the FP7 project on data mining called e-LICO (e-Laboratory for Interdisciplinary Collaborative Research in Data Mining and Data-Intensive Sciences) where we developed new web services for subgroup discovery.

We successfully concluded our collaboration within the FP7 project PHAGOSYS (Systems biology of phagosome formation and maturation - modulation by intracellular pathogens), where we used equationdiscovery approaches to learn models of the dynamics of endocytosis, an important process of immune response, and analyzed high throughput data from compound and genomic screens about different aspects of the same process (e.g., in response to different pathogens). We continued our collaboration in two other FP7 projects: SUMO, where we are developing methods for learning supermodels (ensemble models of dynamic systems), and REWIRE, where we apply machine-learning methods to analyze patient-record and sensor data in the context of post-stroke rehabilitation. In September we started work on the EU 7FP FET project from the field of computer understanding of natural language called MUSE (Machine Understanding for interactive StorytElling), the goal of which is to illustrate texts as 3D animation. In the area of text and web mining and heterogeneous information network analysis we continued our research in Rule Learning" (Springer 2012, 334 the framework of three European FP7 projects: FIRST (Large scale information extraction and integration pages), co-authored by Prof. Nada Lavrač, infrastructure for supporting financial decision making), FOC (Forecasting Financial Crises), and ENVISION (ENVIronmental Services Infrastructure with ONtologies). In FIRST and FOC we focus on analyzing large amounts of dynamic and heterogeneous sources of financial information and develop online data-mining and modern data mining.

We produced the first digital dictionary of historical Slovene, containing over 20,000 entries and available from http://nl.ijs.si/imp/, which can be used by linguists, as well as for applications in human language technologies, e.g., to support a full-text search in digital libraries of Slovenian cultural heritage.

Springer Figure 1: Monograph "Foundations of presents the foundations, techniques and selected applications of rule learning as investigated in classic machine learning

hannes Fürnkran an Gamberg

Foundations of

Rule Learning







Figure 2: Result of successful EU FP7 project BISON is an open-access book "Bisociative Knowledge Discovery", Springer 2012. Members of the Department of Knowledge Technologies at JSI contributed nine book chapters addressing methods for discovering new, domain-bridging connections and patterns from heterogeneous data sources. tools for near-real-time processing of vast amounts of constantly evolving data (financial news, blogs and tweets). We permanently monitor 200 financial websites and capture about 40,000 documents per day. In 2012 we focused on data analysis and end-user solutions, such as sentiment analysis on financial products, estimating the reputation of financial institutions, and on online fraud detection. In FOC we extract indicators based on the sentiment analysis of large streams of textual data with the goal of forecasting financial crises. In ENVISION we develop tools for multilingual support for ontology management and a semantic description of geographic data and services. The tools are integrated into a web application and constitute one of the modules of the on-line environmental decision support portal.

During the 2012 Slovenian presidential elections, we launched a novel public sentiment monitoring solution in collaboration with Gama System and POP TV. We developed a sentiment analysis prototype that collected and analyzed tweets about the three presidential candidates. The sentiment charts were shown on prime time during live TV debates on POP TV and were controversial in the sense that they were in conflict with the polls carried out by the major polling agencies in Slovenia. The polling agencies predicted the then-current president would win the first round of elections, while our system clearly showed the lead of Borut Pahor, who in the end won both the first and the final round of elections.

In the area of language technologies we continued work on the development of language resources and technologies for historical Slovene, where we produced a manually annotated corpus (300,000 words), a digital lexicon (20,000 entries) and an annotation tool for historical Slovene, with which we then annotated a large collection (400 books, 30,000 pages) of historical Slovene texts and made it available as a digital library and through a web-based concordancer. With this we are enabling empirically based studies of diachronic Slovene, as well as better accessibility of Slovene written cultural heritage, already used in the dLib.si digital library portal of the National and University Library (NUL) of Slovenia. This work was undertaken in the scope of the FP7 project IMPACT (Improving Access to Text) in which we collaborate with NUL and as part of the Google awarded project "Developing language models for historical Slovene", in which we collaborate with the Scientific Research Centre of the Slovene Academy of Sciences and Arts (SRC SASA). In the scope of the national project "Unknown 17th and 18th century manuscripts of Slovene

literature: information-technology aided register, scholarly editions and analyses" we finished our joint work with SRC SASA, where we implemented a Fedora Commons platform for searching manuscript descriptions and viewing manuscripts. We also started joint work with SRC SASA on the national project "Leading Slovene Humanists from the 16th to the mid-19th Century".

In the scope of the project "Communication in Slovene", under the lead of the company Amebis we finished work on a new generation of reference corpora for Slovene (e.g., Gigafida with more than a billion words), which also include large freely available corpora, so far lacking for the Slovene language. We completed our work on the linguistic annotation of parallel bi-lingual corpora, performed in the scope of the national project "Slovene transla-

Launch of a novel, public sentiment monitoring system in collaboration with Gama System and POP TV, aired in prime time during the 2012 presidential elections.



Figure 3: Twitter sentiment about candidates at the 2012 Slovenian presidential elections shown on POP TV. Source: http://www. predsedniskevolitve.si/, Gama System in collaboration with Jožef Stefan Institute, Slovenia.

tion studies – resources and research" under the lead of the Department for Translation Studies at the Arts Faculty of the University of Ljubljana. The corpora are used for linguistic studies of translation processes, while also being useful for the development of multilingual language technologies. In cooperation with the same department we are continuing work on enlarging and cleaning the Slovene semantic lexicon sloWNet, where we collaborated in the development of two tools: sloWTool, a browser and editor for sloWNet, and sloWCrowd, a crowdsourcing tool for lexicon cleaning. In 2012 we started with work on implementing web services to linguistically annotated texts; so far we have implemented part-of-speech tagging and lemmatization for Slovene and English in the workflow construction environments Orange4WS and ClowdFlows.

We collaborated in the work of the Slovene Institute of Standardization, as the Slovene delegates of ISO/TC37/SC4 "Terminology and Other Language and Content Resources / Language Resources Management" by taking part in the meetings of ISO TC 37 and in reviewing, translating and approving Slovene standards from this field. We were active in the preparation of the National Program for Language Policy 2012-2016 and in taking the steps necessary for Slovenia to join the research infrastructure CLARIN (Common Language Resources and Technology Infrastructure) at the Slovene Ministry of Culture.

In the area of decision support our long-term goal is to develop methods and techniques of decision modeling, support them with software and inte-

grate them with data-mining systems. In 2012 we developed a new version (3.04) of the computer program for multi-attribute decision-making DEXi, which brings better reporting capabilities and completely re-implemented JDEXi, a java library for the evaluation of decision alternatives. We also improved existing and developed new methods for the ranking of alternatives in qualitative multi-attribute models, based on copulas, which improve the sensitivity of decision models and alleviate some drawbacks of existing methods. In the framework of the 7FP EU project e-LICO, we developed a multi-attribute model for the evaluation of workflows in Rapid Miner, a wellknown data-mining suite. In the 7FP project FIRST, we started the development of evaluation models for banking and finance. We developed a model for the assessment of roof coverings, which is methodologically interesting for its explicit modeling of context-based dependencies. Our results on six decision-support models related to growing and using genetically-modified crops, which were achieved in the already finished EU 7FP project Co-Extra, were published in 2012 in a Wiley-Blackwell book.

We participated in the project EVADIFF (Evaluation et de développement et modèles outils d'aide à la décision utilisés pour la Prevention des pollutions diffuses par les produits phytopharmaceutiques), commissioned by ARVALIS Institut du Vegetal, France, where we develop a decision-support system for the selection of mitigation measures for the protection of surface waters from pollution by phytopharmaceuticals.

Some outstanding publications in the past year

- Stojanova, D., Ceci, M., Appice, A., Džeroski, S.: Network regression with predictive clustering trees. Data mining and knowledge discovery, 2012, vol. 25, no. 2, pp. 378–413
- Grčar, M., Trdin, N., Lavrač, N.: A methodology for mining documentenriched heterogeneous information networks. Comput. j., [in press] 2012, 15 pages
- Aho, T., Ženko, B., Džeroski, S., Elomaa, T.: Multi-target regression with rule ensembles. J. mach. learn. res., [Print ed.], 2012, vol. 13, pp. 2367–2407
- Miljković, D., Stare, T., Mozetič, I., Podpečan, V., Petek, M., Witek, K., Dermastia, M., Lavrač, N., Gruden, K.: Signalling network construction for modelling plant defence response. PloS one, 2012, vol. 7, no. 12, pp. e51822-e51822-18. http://ponta.ijs.si/mozetic/papers/Miljetalsignet-PlosONE-12.pdf
- Logar Berginc, N., Grčar, M., Brakus, M., Erjavec, T., Arhar Holdt, Š., Krek, S.: Korpusi slovenskega jezika Gigafida, KRES, ccGigafida in ccKRES: gradnja, vsebina, uporaba, (Zbirka Sporazumevanje). 1. izd. Ljubljana: Trojina, zavod za uporabno slovenistiko: Fakulteta za družbene vede, 2012. 208 pages, ilustr. ISBN 978-961-92983-6-7. ISBN 978-961-235-596-8
- Mileva-Boshkoska, B., Bohanec, M: A method for ranking non-linear qualitative decision preferences using copulas. International journal of decision support system technology, [in press] 2012, 17 pages

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Figure 4: User interface for a system for the automatic annotation of microscopic diatom images. The query image and the reported identification results (taxon name and probability) are shown in the upper part. The bottom part shows the reference images for the identified taxon name that are present in the database.

Nada Lavrač gave an invited lecture at The 25th IEEE International Symposium on Computer-Based Medical Systems - CBMS 2012, held in Rome in June 2012.



Figure 5: The first digital dictionary of historical Slovene, containing over 20,000 entries and available from http://nl.ijs.si/imp/, can be used by linguists, as well as for applications in human language technologies, e.g., to support full-text search in digital libraries of Slovenian cultural heritage.

Organization of conferences, congresses and meetings

- The 22nd International Conference on Inductive Logic Programming ILP 2012, Dubrovnik, Croatia, 17.–19.
 9. 2012
- Subconference: Intelligent Systems, and Conference on 100 Years of Alan Turing and 20 Years Of SLAIS, Information Society 2012, Ljubljana, Slovenia 8.–12. 10. 2012
- 3. Project meeting of European project REWIRE, Ljubljana, Slovenia, 17.-18. 9. 2012

INTERNATIONAL PROJECTS

- 1. EVADIFF: Evaluation of existing models and development of new decision-making tools to prevent diffuse pollution caused by plant protection products Arvalis - Institut du Végétal
- Prof. Marko Debeliak
- 7. FP PHAGOSYS: Systems biology of phagosome formation and maturation, 2 modulation by intracellular pathogens European Commission
- Prof. Sašo Džeroski
- 3. 7. FP - ENVISION: Environmental services infrastructures with ontologies European Commission
- Miha Grčar, Prof. Nada Lavrač 4. 7. FP - IMPACT: Improving access to text European Commission
- Asst. Prof. Tomaž Erjavec
- 7. FP FIRST: Large scale information extraction and integration infrastructure for supporting financial decision making
- European Commission Miha Grčar, Prof. Nada Lavrač
- 7. FP e-LICO: E-laboratory for collaborative interdisciplinary research in data mining 5. and data intensive sciences European Commission
- Prof. Nada Lavrač, Asst. Prof. Martin Žnidaršič
- 7. FP SUMO: Supermodeling by combining imperfect models 6. European Commission
- Prof. Sašo Džeroski 7. FP - FOC-II: Forecasting financial crises
- European Commission Dr. Igor Mozetič, Miha Grčar
- 7. FP REWIRE: Rehabilitative wayout in responsive home environments 7 European Commission
- Prof. Sašo Džeroski, Asst. Prof. Bernard Ženko
- 8 7. FP - MUSE: Machine understanding for interactive storytelling European Commission Prof Nada Lavrač
- COST IC1002, MUMIA: Multilingual and multifaceted interactive information access 9 COST Office

Dr. Igor Mozetič, Asst. Prof. Tomaž Erjavec

VISITORS FROM ABROAD

- Dr. Ivica Dimitrovski, Faculty of Electrical Engineering and Information Technologies, 1. University Ss. Cyril and Methodius, Skopje, Macedonia, 8.-29. 1. 2012
- Dr. Gjorgji Madjarov, Faculty of Electrical Engineering and Information Technologies, 2 University Ss. Cyril and Methodius, Skopje, Macedonia, 8.-29. 1. 2012
- 3 Dr. Nikola Ljubešić, Univerza v Zagrebu, Zagreb, Croatia, 6.-9. 2. 2012
- Prof. dr. Suzana Loškoska, Faculty of Electrical Engineering and Information 4.
- Technologies, University Ss. Cyril and Methodius, Skopje, Macedonia, 1. 3.-1 10. 2012 5 Akad. prof. dr. Ljupčo Kocarev, Macedonian Academy of Sciences and Arts, Skopje, Macedonia, 11.-16. 3. 2012
- 6. Dr. Michelangelo Ceci, Universita degli Studi di Bari, Bari, Italy, 23.-25. 4. 2012
- Dr. Michelangelo Puliga, ETH, Zurich, Switzerland, 15.-18. 5. 2012, 18. 12. 2012
- Dr. Dragan Gamberger, Rudjer Bošković Institute, Zagreb, Croatia, 15.-18. 5. 2012 8.
- Dr. Tomislav Šmuc, Rudjer Bošković Institute, Zagreb, Croatia, 15.-18. 5. 2012, 15. 11. 2012 9.
- 10 Nino Antulov Fantulin, Rudjer Bošković Institute, Zagreb, Croatia, 15.-18. 5. 2012, 18.12.2012
- 11. Matija Piškorec, Rudjer Bošković Institute, Zagreb, Croatia, 15.-18. 5. 2012, 15. 11. 2012

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- Prof. Marko Bohanec
- Prof. Bojan Cestnik* Prof. Marko Debeljak 3.
- Prof. Sašo Džeroski 4.
- 5. Asst. Prof. Tomaž Erjavec
- Prof. Nada Lavrač, Head 6.
- Prof. Tanja Urbančič
- Postdoctorial associates
- 8. Dr. Dragi Kocev Dr. Petra Kralj Novak
- 10. Dr. Panče Panov
- 11. Dr. Ivica Slavkov

- 10. The European network on word structure ESF - European Science Foundation Asst. Prof. Tomaž Erjavec
- 11. Identifying optimal management strategies for biodiversity and related ecosystem services on private forests Slovenian Research Agency Prof. Marko Debeljak

RESEARCH PROGRAM

1. Knowledge Technologies Prof. Nada Lavrač

R & D GRANTS AND CONTRACTS

- 1. Systemic biology approaches to analyzing interactions between pathogens and plants Prof. Nada Lavrač
- 2. Slovene translation studies - resources and research Asst. Prof. Tomaž Erjavec 3
 - Growth and defense trade-offs in multitrophic interaction between potato and its two major pests
 - Prof. Nada Lavrač
- 4. The leading humanists in the Slovenian territory between the 16th and mid-19th centuries and their social and cultural environment Asst. Prof. Tomaž Erjavec
- Data mining for integrative data analysis in systemic biology
- Prof. Sašo Džeroski
- 6. Semantic rule discovery in the context of Web services Prof. Nada Lavrač
- Ecological restoration of natural disturbances in forests 7 Prof. Marko Debeljak
- 8 Google digital humanities award for developing language models for historical Slovene Asst. Prof. Tomaž Eriavec
- 22nd International conference on inductive logic programming Dubrovnik ILP 2012, 17.-19.9.2012. Dubrovnik Prof Nada Lavrač
- 12. Marko Popović, Rudier Bošković Institute, Zagreb, Croatia, 15,-18, 5, 2012, 4,-5, 11. 2012, 4.-5. 12. 2012
- Dražen Lučanin, Rudjer Bošković Institute, Zagreb, Croatia, 15.-18. 5. 2012 13.
- Prof. dr. Benedict Brors, German Cancer Research Center DKFZ, Heidelberg, Germany, 14 25 - 27 7 2012
- 15. Dr. Florence Leprince, ARVALIS Institut du végétal, Montardon, France, 6. 8. 9. 2012, 7-8 11 2012
- 16. Dr. Barry Hardy, Douglas Connect, Zeiningen, Switzerland, 5. 5. 2012
- Richard Wheeler, University of Edinburgh, Edinburgh, Scotland, 4.-9. 9. 2012 17
- Prof. dr. Hiroshi Motoda, AFOSR/AOARD in University of Osaka, Osaka, Japan, 18. 19.-23.9.2012
- Prof. dr. João Gama, University of Porto, Laboratory of Artificial Intelligence and 19 Decision Support, and Faculty of Economics, Porto, Portugal, 8.-14. 10. 2012
- 20. Dr. Nataša Pržulj, Imperial College, London, UK, 6. 11. 2012
- 21. Dr. Benoit Real, ARVALIS Institut du végétal, Paris, France, 7.-8. 11. 2012
- 12. Dr. Aneta Trajanov
- 13. Asst. Prof. Bernard Ženko
- 14. Asst. Prof. Martin Žnidaršič
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- 16. Miha Grčar, B. Sc. 17. Dr. Elena Ikonomovska
- 18. Matjaž Juršič, B. Sc.
- 19. Janez Kranjc, B. Sc.
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- 21. Matic Perovšek, B. Sc.
- 22. Vid Podpečan, B. Sc.
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 Anže Vavpetič, B. Sc.
 Technical officers
 Marko Brakus, B. Sc., left 01.05.12

29. Dr. Igor Mozetič

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ORIGINAL SCIENTIFIC ARTICLE

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- 2. Darko Čerepnalkoski, Katerina Taškova, Ljupčo Todorovski, Nataša Atanasova, Sašo Džeroski, "The influence of parameter fitting methods on model structure selection in automated modeling of aquatic ecosystems", In: Proceedigs of the 7th ECEM, European Conference on Ecological Modelling, 30 May 2 June 2011, Riva el Garda, Italy, *Ecol. Model.*, vol. 245, pp. 136-166, 2012.
- 3. Marko Debeljak, Aneta Trajanov, Daniela Stojanova, Florence Leprince, Sašo Džeroski, "Using relational decision trees to model out-crossing rates in a multi-field setting", In: Proceedigs of the 7th ECEM, European Conference on Ecological Modelling, 30 May - 2 June 2011, Riva el Garda, Italy, *Ecol. Model.*, vol. 245, pp. 75-83, 2012.
- Ivica Dimitrovski, Dragi Kocev, Suzana Loskovska, Sašo Džeroski, "Hierarchical classification of diatom images using ensembles of predictive clustering trees", *Ecological informatics*, vol. 7, no. 1, pp. 19-29, 2012.
- 5. Tomaž Erjavec, "Jezikoslovni viri starejše slovenščine", In: Ljubljana v BiTiH - BiTi v Ljubljani: prispevki iz prvega ljubljanskega kongresa digitalizacije kulturne dediščine = papers from the first Slovenian congress for digitisation of cultural heritage: tematska številka, (Knjižnica, 56, 3), Ines Vodopivec, ed., Ljubljana, Zveza bibliotekarskih društev Slovenije, Narodna in univerzitetna knjižnica, 2012, pp. 205-221.
- 6. Tomaž Erjavec, "MULTEXT-East: morphosyntactic resources for Central and Eastern European languages", *Language resources and evaluation*, vol. 46, no. 1, pp. 131-142, 2012.
- Frieder Graef *et al.* (38 authors), "A framework for a European network for a systematic environmental impact assessment of genetically modified organisms (GMO)", *BioRisk (Print)*, vol. 7, pp. 73-97, 2012.
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 Marko Lazar, Using web technologies for marketing communication in sport: master's thesis, Nova Gorica, 2012 (mentors Bojan Cestnik, Tanja Urbančič).
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DEPARTMENT OF INTELLIGENT SYSTEMS

The Department of Intelligent Systems develops new methods and techniques for intelligent computer systems, with applications in the areas of the information society, computer science and informatics, and network communication systems. The main research areas are ambient intelligence, computational intelligence, agent modeling, and language and speech technologies. The department collaborates closely with the Faculty of Computer and Information Science of the University of Ljubljana on the joint research program "Artificial Intelligence and Intelligent Systems", led by Prof. Ivan Bratko.

Intelligent systems simulate intelligence so that a typical user perceives them as truly intelligent. However, in reality, these systems use complex mechanisms and implement them on digital computers to imitate human behavior as well as possible, exploiting raw, exponentially growing computer power.

Ambient intelligence is an increasingly important research area aiming to introduce the technology into our everyday environment in a friendly way that is undemanding for the user. The two key topics of ambient intelligence Head: we work on are (1) telemedicine and elderly care, and (2) smart buildings. The European telemedicine project CHI- Prof. Matjaž Gams RON is concerned with monitoring chronic heart-disease patients at home. Our task is activity recognition and the estimation of the patient's energy expenditure with accelerometers. Additionally, we worked on a decision-support system for the physicians to assess the risk to the patient's health. Since activity recognition is one of the fundamental

tasks of ambient intelligence, we upgraded the activity recognition from the CHIRON project into the TriLAR (three-layer activity recognition) method. Another important task is the detection of unusual and suspicious behavior, which we tackled in a doctoral research project. When analyzing human behavior, it is important to adapt to each individual user. For this purpose we developed a semi-supervised learning method called MCAT (multi-classifier adaptive training). Finally, we worked on the recognition of typical diseases

of the elderly and fall detection. In the ELKOV22 project we cooperate with the Elgoline, Kovinoplastika and INTECH-LES razvojni center companies to develop an intelligent door system. In the door we integrated an intelligent system

consisting of sensors, actuators, controllers, communication interfaces and mobile applications. The system provides smart functionalities devoted to comfort (voice messages, event monitoring, remote control) and security (detection of movement and banging on the door, alarms with images over e-mail or SMS, etc.). The most advanced functions are the recognition of unusual entries/exits, automatic identification/verification of the entering individuals, a user interface featuring a virtual assistant, and learning the habits of the inhabitants to optimize the energy consumption of the building. In the area of smart buildings we were also developing a multi-agent building-control system with the purpose of performing a multi-objective optimization of comfort and energy consumption.

Computational intelligence is a study of stochastic search, optimization and learning methods, inspired by physical and biological systems. Research in this area at the Department of Intelligent Systems focuses on evolutionary computation methods. We study extensions of evolutionary algorithms for multiobjective optimization and their speedup, and apply these algorithms in engineering design and optimization problems. In doctoral research projects, we develop a method for the visualization of multidimensional fronts of nondominated solutions in multiobjective optimization, an algorithm for the discovery of optimal car-driving strategies with respect to the traveling time and the fuel consumption, and optimization based on surrogate models. In addition, our work is motivated by the optimization of metallurgical production processes, which is a subject of two research projects executed together with the University of Nova Gorica, In the European project CHIRON we monitor chronic heart-disease patients at home. The recognized patient's activity and estimated energy expenditure represent the context for the observation of the patient's heartbeat.

Figure 1: An intelligent door system, developed in cooperation with the INTECH-LES razvojni center and companies Kovinoplastika Lož and Elgoline, was demonstrated at the Ambient furniture fair from 6th to 11th November 2012, and presented in a short interview on RTV Slovenia.

ЧГ



E-9



e-vratar



Figure 2: Visualization of three 4D Pareto front approximations in 3D using prosections

In the ELKOV22 project we cooperate with industrial partners to develop an intelligent-door system. The project is focused on the security and the detection of unusual events during entrance.



Figure 3: At the 5th International Conference on Bioinspired Optimization Methods and their Applications – BIOMA 2012, held in Bohinj, Slovenia, on 24 and 25 May 2012, 30 papers by 70 (co)authors from 13 countries were presented.

The goal of the 7th Framework Program project MIRABEL is to develop a computer infrastructure to efficiently balance the generation and consumption of electrical energy for an increased amount of energy from renewable sources. Institute of Metals and Technology, Ljubljana, and the Štore Steel company. A substantial part of our applied research is devoted to energy efficiency. In collaboration with partners from five European countries, we carry out the 7th Framework Program project **MIRABEL** (originally MIRACLE). Its goal is to develop a computer infrastructure to efficiently balance between the generation and consumption of electrical energy for an inreased amount of energy from renewable sources. This infrastructure relies on flexible offers for energy generation and consumption, their aggregation and scheduling. For this project we implemented scheduling algorithms for assigning the time and energy amount to the offers.

In the field of **agent modeling** we are focused on the behavior analysis and cloning of individuals and groups. Most of the work is performed for the **EUSAS** project, which is funded by the European Defense Agency. The aim is to develop a new approach to mission training for low-level units (security, police force, etc.) facing asymmetric threats in an urban environment. The developed tools can be used to discover the common agent strategy by knowing only low-level agent behavior and possessing basic domain knowledge. The discovered strategic action descriptions are presented to the user in the form of graph paths, agent actions, roles and corresponding rules. The rules, constructed by machine learning, enrich the graphical strategic patterns and describe the conditions under which individual actions present in the pattern occur. Moreover, meaningful behavior patterns are later used during behavior cloning, where software agents reproduce the observed behavior of real operational people. Experiments have shown that the developed approach allows for a high-quality reproduction of behavior.

In the field of **speech and language technologies** we work on speech synthesis, forensic speaker recognition, semantic analysis of text and question answering. Together with the Amebis company, we are developing a new speech synthesizer for Slovene. Special attention is paid to the requirements of elderly, handicapped and visually impaired people. In cooperation with the national television and radio, RTV Slovenia, we recorded a phonetically rich and balanced speech database for corpus-based speech synthesis. In speaker recognition we continue to investigate the correlation between the speech quality in telephony and the performance of automatic speaker verification.

In collaboration with the Department of Computer Systems, we organized the 5th International Conference on Bioinspired Optimization Methods and their Applications – BIOMA 2012, held in Bohinj, Slovenia, on 24 and 25 May 2012, and devoted to theoretical and practical aspects of optimization methods based on the models of biological processes and associations. There were 30 papers by 70 (co)authors from 13 countries presented at the conference. The invited lecturers were Prof. Ágoston E. Eiben from VU University of Amsterdam, and Dr. Xin-She Yang, from the National Physical Laboratory in Teddington, UK.

From 8 to 12 October 2012, the 15th International Multiconference Information Society – IS 2012 took place at the Jožef Stefan Institute. It consisted of ten independent conferences with 215 papers. The special event was the conference "100 Years of Alan Turing and 20 Years of SLAIS" gather-

ing scientists that had a significant impact on the field of artificial intelligence in the past decades. Four conference awards were given: for exceptional contribution to the development and promotion of the information society, for current achievements in the field of information society, and the information strawberry and lemon for the best and worst public information-society services.

Some outstanding publications in the past year

1. Kaluža, B., Gams, M.: Analysis of daily-living dynamics. Journal of Ambient Intelligence and Smart Environments, 2012, 4(5), pp. 403-413

- Korošec, P., Šilc, J., Filipič, B.: The differential ant-stigmergy algorithm. Information Sciences, 2012, 192, pp. 82–97
- Luštrek, M., Bratko, I., Gams, M.: Independent-valued minimax: Pathological or beneficial? Theoretical Computer Science, 2012, 442, pp. 59–77
- Marinčič, D., Šef, T., Gams, M.: Parsing with clause and intraclausal coordination detection. Computing and Informatics, 2012, 31(2), pp. 299–329
- Piltaver, R., Luštrek, M., Gams, M.: The pathology of heuristic search in the 8-puzzle. Journal of Experimental & Theoretical Artificial Intelligence, 2012, 24(1), pp. 65–94
- Pogorelc, B., Gams, M.: Home-based health monitoring of the elderly through gait recognition. Journal of Ambient Intelligence and Smart Environments, 2012, 4(5), pp. 415–428

Organization of conferences, congresses and meetings

- 1. The 5th International Conference on Bioinspired Optimization Methods and their Applications, BIOMA 2012, Bohinj, Slovenia, 24.–25. 5. 2012
- 2. 4th Jožef Stefan International Postgraduate School Students Conference, Jožef Stefan Institute, Ljubljana, 25. 5. 2012
- 20th Workshop on Nature-Inspired Algorithms, AVN, Šmarna gora, Slovenia, 20. 9. 2012
- 15th International Multiconference Information Society, IS 2012, 8.–12.
 2012; independent conferences: 100 Years of Alan Turing and 20 Years of SLAIS, Intelligent Systems, Data Mining and Data Warehouses (SiKDD 2012), Collaboration, Software and Services in Information Society, Cognitive Sciences, Robotics, Language Technologies, Education in Information Society, FORSEE Technological Forecasting in ICT, Facing Demographic Challenges

INTERNATIONAL PROJECTS

- 1. 7. FP MIRACLE, MIRABEL: Micro-request-based aggregation, forecasting and scheduling of energy demand, supply and distribution European Commission
- Prof. Bogdan Filipič
 2. 7. FP Xperience: Robots bootstrapped through learning from experience European Commission
- Prof. Matjaž GamsEUSAS: European urban simulation for asymmetric scenarios EADS N.V., Defense And Security Systems
- Prof. Matjaž Gams
 Constrained multiobjective optimization based on simulation models Slovenian Research Agency
 Prof. Bogdan Filipič

RESEARCH PROGRAM

1. Artificial intelligence and intelligent systems Prof. Matjaž Gams

R & D GRANTS AND CONTRACTS

1. Advanced modelling and simulation of liquid-solid processes Prof. Bogdan Filipič

- Simulation and optimization of casting, rolling and heat treatment processes for competitive production of topmost steels Prof. Bogdan Filipič
- 3. The 15th international multiconference Information Society 2012
- Prof. Matjaž Gams 4. Open communication platform for service integration
- Prof. Matjaž Gams 5. E-Reader in Slovene for the blind and visually impaired
- E-Reader in Slovene for the blind and visually impaired Dr. Tomaž Šef
- Crowdsourcing support for reassembly of wall painting fragments Prof. Bogdan Filipič
- 7. Electronic mobile tourist guide
- Dr. Mitja Luštrek
- 8. Virtual assistant for municipalities and societies Prof. Matjaž Gams
- ARTEMIS, CHIRON: Cyclic and person-centric health management: Integrated approach for home, mobile and clinical environments Dr. Mitja Luštrek

NEW CONTRACTS

- 2nd project phase: Intelligent surveillance and administration system for wooden residences
- Intech Les, d. o. o.
- Prof. Matjaž Gams
- 2. Development of virtual assistant
 - Education, Science and Culture Trade Union of Slovenia Prof. Matjaž Gams



Figure 4: An example of a discovered strategic behavior pattern. The pattern is composed of a graphical (sequences of actions) and symbolic part (rules).

The main goal of the EUSAS project is to develop a new approach to mission analysis and training for low-level units facing asymmetric threats in an urban environment.

VISITORS FROM ABROAD

- Prof. Erkki Laitinen, University of Oulu, Department of Mathematical Sciences, Oulu, 1. Finland, 20.-26. 5. 2012
- Martin Gjoreski, Faculty of Computer Science and Engineering, Univerzitet Sv. Kiril in 2. Metodij, Škopje, Macedonia, 1.–31. 8. 2012 Dr. David Križaj, Department of Ophthalmology and Visual Sciences, University of
- 3. Utah, Utah, USA, 5.-23. 10. 2012
- 4 Prof. Adam Przepiorkowski, Institute of Computer Science, Polish Academy of Sciences, Warsaw, Poland, 6.–9. 10. 2012
- 5 Prof. Liliana Albertazzi. Center for Mind and Brain Sciences. University of Trento. Trento, Italy, 7.-11. 10. 2012
- Luisa Milic, Ideya Business and Marketing Consultancy, Cambridge, United Kingdom, 6 7-11 10 2012
- Dr. Albert Bifet, University of Waikato, Hamilton, New Zealand, 8.-11. 10. 2012

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- Dr Mitia Luštrek 5
- 6.
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- 10. Dr. Matej Guid*
- 11. Dr. Aleksander Pivk* 12. Dr. Vedrana Vidulin
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13. Robert Blatnik, M. Sc.

- 14. Božidara Cvetković, B. Sc.
- 15. Erik Dovgan, B. Sc.
- 16. Boštjan Kaluža, B. Sc.
- 17. Tomaž Kompara*, B. Sc.
- 18. Simon Kozina, B. Sc.

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ORIGINAL SCIENTIFIC ARTICLE

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- Prof. Marko Tadić, Faculty of Arts, University of Zagreb, Zagreb, Croatia, 8.-12. 10. 2012 10. Prof. Joao Gama, Laboratory of Artificial Intelligence and Decision Support, Porto, Portugal, 11. 10. 2012
- Dr. Nataša Milić Frayling, Microsoft Research Cambridge, Cambridge, United Kingdom, 11 11 10 2012
- 12. Prof. Gerhard Friedrich, Intelligent Systems and Business Informatics, Universität Klagenfurt, Klagenfurt, Austria, 11.-12. 10. 2012
- 13 Dr. Gerald Steinbauer, Institute for Software Technology, Graz University of Technology, Graz, Austria, 11.-13, 10, 2012
- 14. Prof. Claude Sammut, University of New South Wales, Kensington, Australia, 16. 10. 2012
- 19. Jana Krivec*, B. Sc. 20. Damjan Kužnar, B. Sc. 21. Violeta Mirchevska* 22. Miha Mlakar, B. Sc. 23. Rok Piltaver, B. Sc. 24. Bogdan Pogorelc*, B. Sc. Aleš Tavčar, B. Sc. 25 26. Tea Tušar, M. Sc. 27. Domen Zupančič** Technical officers 28. Mitja Kolbe*, B. Sc. 29. Gašper Pintarič*, B. Sc. Technical and administrative staff 30. Dr. France Dacar, retired 29.07.12 31. Vesna Koricki Špetič, B. Sc. 32. Mitja Lasič 33. Liljana Lasič 34. Lana Zemljak Note
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PATENT APPLICATION

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MENTORING

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- Vedrana Vidulin, Searching for credible relations in machine learning: doctoral dissertation, Ljubljana, 2012 (mentor Matjaž Gams; comentor Bogdan Filipič).
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DEPARTMENT OF REACTOR ENGINEERING

R-4

The Department of Reactor Engineering is involved in basic and applied research in the fields of nuclear engineering and safety. Topics include the modelling of basic thermal-hydrodynamic phenomena, thermal-hydraulic safety analyses of design-basis and severe accidents, structural safety analyses and probabilistic safety assessments. Most research activities are part of international cooperation programs. The research results are incorporated in projects for industry and for the regulatory authorities, as well as in under-graduate and doctoral studies programmes.

Modelling of basic thermal-hydrodynamic phenomena

Modelling of the underlying mechanisms of convective boiling and critical heat flux was carried out in the frame of the NURISP project (EC, 7th FP). The modelling accuracy of the bubble departure diameter in boiling was calculated by applying an uncertainty analysis method on the analytical model for bubble growth, where the uncertainties of the wetting angle and surface tension were considered. Within the research on critical heat flux, a local model for boiling crisis initiation was developed.

Turbulent flow modelling is used in research related to the development of future fission and fusion reactor Prof. Leon Cizelj systems. We performed direct numerical simulations of turbulent heat transfer in channels at the Prandtl number 0.01. These simulations took into account heat conduction in the fuel and enabled a detailed analysis of temperature fluctuations inside the fuel, which are induced by turbulent flow. The research was carried out within the THINS project (EC, 7th FP) and is relevant for next-generation fission reactors that will be cooled with liquid sodium.

Simulations of the blind benchmark test MATIS-H (Korea Atomic Energy Research Institute - KAERI) were carried out in the frame of an OECD/NEA project. The test represents turbulent flow through a horizontal fuel bundle grid with mixing vanes. A highly turbulent swirl flow was simulated with the ANSYS CFX and OpenFOAM codes. Our simulation results showed a good agreement with experimental data and were ranked among the most accurate on the international level.

For the past few years the department has been actively involved in the development of the helium-cooled diverter for the DEMO fusion reactor. In 2012, alternative cooling-finger concepts were investigated and analysed. The results have shown that the diverter can be effectively cooled by using a tantalum alloy and square-shaped finger tiles. Also within the DEMO development, we have studied the possibilities

of coupling the MCNP neutronic analysis with the ANSYS CFX thermalhydrodynamic analysis. Both activities were carried out in collaboration with the Karlsruhe Institute of Technology - KIT (Germany) within the European Fusion Development Association (EFDA).



Head

An experiment on hydrogen combustion in a

240 m³ experimental vessel was performed.

Various transients in single- or two-phase (gas-liquid) flow could occur in the piping systems of nuclear plants during design-basis accidents. The WAHA computer code for simulating transients was further developed: new models of two-phase stratified and slug flow were tested with simulations of condensation-induced water hammer in a horizontal pipe (within the NURISP project). Within a bilateral cooperation with KFKI (Hungary), the WAHA code was also tested at supercritical temperatures and pressures, at which some next-generation nuclear reactors are designed to operate.

An experiment on hydrogen combustion was performed in the HYKA A2 facility at KIT (Germany) within the EC project LACOMECO. The HYKA A2 facility is a cylindrical vessel with a volume of 240 m³. The experiment was proposed and specified by the department, whereas it was executed by KIT staff. A hydrogen-steam-air mixture was ignited at the bottom of the vessel, which caused combustion and flame propagation. The purpose of the experiment was to determine the pressure and temperature increases, as well as the flame-propagation velocity in the radial and vertical directions.

A steam explosion might occur during a hypothetical nuclear accident if the molten reactor core would pour into water. Within the OECD/NEA project SERENA and the SARNET-2 network (EC, 7th FP), we continued simulations and analyses, using the European code MC3D, of steam explosion experiments performed in the KROTOS (Commissariat à l'Energie Atomique - CEA, France) and TROI (KAERI) facilities. We found that melt droplets should be described with multiple droplet-size groups to model the phenomena occurring during the fuel-coolant interaction more adequately. The analysis focused on the influence of melt solidification and oxidation on the explosion strength. In addition, the potential of strong vapour explosions during the melt-sodium interaction was investigated.

Thermal-hydraulic safety analyses

The advanced TRAC/RELAP Advanced Computational Engine (TRACE), developed by the U.S. Nuclear Regulatory Commission, enables a multidimensional description of the physical phenomena and processes in reactor systems. A three-dimensional (3D) TRACE input model of the BETHSY facility (CEA, France) was developed, with a 3D reactor vessel model, while the models of other components are one-dimensional. The first 3D simulations of the BETHSY 9.1b and 6.2TC tests (2-inch and 6-inch cold leg break without high-pressure safety injection) were performed. The accuracy of the calculated results, as assessed using the fast-Fourier-transform-based method (FFTBM) for the



Figure 1: Numerical simulation of turbulent flow through a horizontal fuel bundle in a grid with mixing vanes.

BETHSY 6.2TC test, was excellent.

In the field of modelling containment phenomena, we participated in the following benchmark exercises within the SARNET-2 network:

Combustion benchmark, where we simulated experiments on hydrogen combustion, performed in the ENACCEF facility at the ICARE centre (France), with the lumped-parameter CONTAIN code.

Condensation benchmark, where we simulated experiments on steam condensation, performed in the CONAN facility at the University of Pisa (Italy), with the CFX code.

Generic containment benchmark, where we simulated a hypothetical transient in an idealized model of a NPP containment with the severe accident ASTEC code.

Structural safety analyses

Recent research has been focused on the development of multiscale computational simulation tools for polycrystalline metallic materials. An advanced constitutive model of crystal plasticity is combined with random grain sizes and shapes. The data on crystal grains are retrieved either from experimental (e.g., X-ray diffraction contrast tomography) or analytical (e.g., Voronoi tessellation) methods. The loading of randomly shaped and oriented crystal grains with anisotropic properties results in highly inhomogeneous microscopic stress fields, which are estimated using the finite-element solver ABAQUS.

In 2012 we proposed and investigated a possible approach for modelling the progressive damage along the grain boundaries of a polycrystalline metal. Explicit finite-element models have been developed which represent

We have proposed a simple constitutive model of anisotropic plasticity that provides faster simulations of the micromechanical response of stainless steel under plastic deformation. the grain boundaries with a cohesive-based surface approach that omit individual cohesive elements and are implemented through the interaction of cohesive surfaces. The results proved the cohesive surfaces to be more accurate and reliable since their influence on the neighbouring grain mesh elements appear to be weaker and much more stable. The results of the analyses also highlighted several other issues related to the computation of

the stresses on cohesive elements. The most severe issue was found within the plastic grain response, where the computed normal stresses could be significantly underestimated.

We have also proposed a simple constitutive model of anisotropic plasticity, which provides faster simulations of the micromechanical response of stainless steel under plastic deformation. We calibrated the model by analysing and comparing the evolution of the in-grain crystal orientations with electron backscatter diffraction measurements. We have found a clear correlation between the computed average scatter of the in-grain orientations and the applied plastic strain. The development of the simulation method benefits from the collaboration with the EC Joint Research Center in Petten (The Netherlands).

A new approach to predicting the thermal fatigue of piping containing the intensive turbulent mixing of fluids with different temperatures has also been developed. We have expanded the analyses of the usual one-dimensional approach, where the distribution of temperatures of the pipe wall is assumed only along the thickness, to a two-dimensional approach, where axial temperature variations are also considered. The results show that the temperature distributions from the one-dimensional approach are more conservative in the prediction of thermal stresses and that shear stress components at the proximity of the inner pipe surface become significant and should therefore be considered in the fatigue analysis.

Probabilistic safety assessment

The implications of the strengthening of the station-blackout mitigation capability on the safety of a nuclear power plant were assessed. The analysis was done with state-of-the-art deterministic and probabilistic methods and tools applied on the reference models of nuclear power plants. The time extension of the blackout-coping capability results in a delay of the core heat up for at least the extension time interval. The largest weighted decrease

of the core damage frequency, considering the costs for the modification, is obtained for the modification resulting in the extension of the stationblackout coping capability.

An uncertainty analysis of specific ageing rates was conducted using an analytical unavailability model applied for a selected safety system of a nuclear power plant. The obtained results indicate the extent to which the uncertainty of the considered ageing data set influences the performed unavailability calculations.

A new method was developed for the explicit modelling of a singlecomponent failure event simultaneously within multiple common-cause failure groups based on a modification of the Beta Factor parametric model.

A multi-objective optimization-based solution to the combined economicenvironmental power dispatch was developed, based on the improved weighted-sum method upgraded with the integration of a new penalty function.

An approach to the reduction of the safety system unavailability with the optimization of the related test and maintenance schedule was also developed. The ageing data uncertainty and test and maintenance costs were considered in the new method.

Technical cooperation, consulting services and education

Reactor Engineering Department researchers also cooperated in projects for industry. As an authorized institution for radiation and nuclear safety, and in the framework of regular Krško nuclear power plant (NPP) activities for maintenance and improvements to nuclear safety, we performed an independent expertise on a plant modification

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related to alternative emergency power supply with the installation of the third diesel generator. During the regular Krško NPP outage, we performed inspection activities on safety structures, systems and components. We prepared a report with proposals for safety improvements.

In preparation for the eventual construction of the second unit of the Krško NPP, we prepared, for the utility company "GEN energija", a com-

prehensive review and description of severe accident management in potential candidate reactors. The following generation III pressurized-water reactors were considered: AP1000, EPR, APWR and ATMEA1.

Members of the department are also actively involved in nuclear engineering under-graduate, masters and doctoral studies at the Faculty of Mathematics and Physics at the University of Ljubljana. The programmes are associated with the European Nuclear Education Network (ENEN) and the European project ENEN-III.

Some outstanding publications in the past year

- 1. Končar, B., Matkovič, M., Prošek, A.: NEPTUNE_CFD analysis of flow field in rectangular boiling channel, Journal of Computational Multiphase Flows, 2012, vol. 4, pp. 399-409
- Uršič, M., Leskovar, M., Mavko, B.: Simulations of KROTOS alumina and corium steam explosion experiments: applicability of the improved solidification influence modelling, Nuclear Engineering and Design, 2012, vol. 246, pp. 163–174
- 3. Tiselj, I., Cizelj, L.: DNS of turbulent channel flow with conjugate heat transfer at Prandtl number 0.01, Nuclear Engineering and Design, 2012, vol. 253, pp. 153–160
- Volkanovski, A.: Method for assessment of ageing based on PSA results, Nuclear Engineering and Design, 2012, vol. 246, pp. 141-146

Awards and appointments

1. Mihaela Uplaznik, Leon Cizelj and Igor Simonovski: The Best Poster Awards, International Conference Nuclear Energy for New Europe 2012, Ljubljana , "Cohesive Based Surface Approach for Grain Boundary Modelling"

Organization of conferences, congresses and meetings

- 1. Cluster workshop project THINS, Ljubljana (JSI Reactor centre), 6. 2.-9. 2. 2012
- 2. TRASNUSAFE Meeting, Ljubljana (JSI Reactor centre), 10. 2. 2012
- 3. SARNET2 WP7-2 & WP7-3 Meeting, Bled, 14. 2.–15. 2. 2012

Figure 2: Distribution of in-grain misorientations in a stainless-steel model under plastic deformation.

The implications of the strengthening of the station-blackout mitigation capability on the safety of a nuclear power plant were assessed.

INTERNATIONAL PROJECTS

- 6. FP NULIFE: Nuclear plant life prediction European Commission Prof. Leon Cizeli
- 7. FP NURISP: Nuclear integrated simulation project European Commission
- Prof. Iztok Tiselj
 7. FP SARNET2: Network of excellence for a sustainable integration of European research on severe accident phenomenology and management phase 2 European Commission
- Dr. Matjaž Leskovar
- 7. FP ÉURATOM ENEN-III: European nuclear education network training schemes European Commission Prof. Leon Cizelj
- 7. FP EURATOM THINS: Thermal-hydraulics of innovative nuclear systems European Commission Prof. Iztok Tiselj
- FP EURATOM TRASNUSAFE: Training scheme on nuclear safety culture European Commission Prof. Borut Mavko
- FP NEWLANCER: New MS linking for an advanced cohesion in Euratom research European Commission Prof. Leon Cizelj
- FP EURATOM, MULTIMETAL: Structural peformance of multi-metal component European Commission
- Prof. Leon Cizelj
 7. FP EURATOM: Modelling of high flux helium cooling divertor design 4.5.1.-FU; Annex 2 to contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Dr. Boštian Končar
- 7. FP MHEST Association: Identification of alternative he-cooled divertor concepts Ministry of Higher Education, Science and Technology Dr. Boštian Končar
- 7. FP EURATOM: Assessment of ANSYS workbench hybrid platform 4.10.1. FU Ministry of Higher Education, Science and Technology Dr. Matjaž Leskovar
- 7. FP EURATOM: Assessment of ANSYS workbench hybrid platform 4.10.1. FU; WP12-DTM-01-T03-01/MHEST/PS
 Misister of United Science of Technology
- Ministry of Higher Education, Science and Technology Dr. Matjaž Leskovar
- 7. FP ÉURATOM, MHEST Association: divertor high flux helium cooling 4.5.1. FU, FU-07-CT-2007-00065 Ministry of Education, Science, Culture and Sport
- Dr. Boštjan Končar 14. Training and tutoring for experts of the NRAs at
- 14. Training and tutoring for experts of the NRAs and their TSOs for developing and strengthening their regulatory and technical capabilities - INSC Project MC.03/10 - LOT 1: training and tutoring for nuclear regulatory authorities and their TSO's ITER-Consult SRL Prof. Leon Cizelj

VISITORS FROM ABROAD

- 1. Gaurang Sharma, Indian Institute of Technology (IIT) Bombay, Mumbai, India, 1. 12. 2011–3. 1. 2012
- 2. I Gusti Agung Wesaka Pu, Embassy of the Republic of Indonesia, Vienna, Austria, 3. 2. 2012
- 3. Dr. Syahril, Nuclear Attache in the Indonesian Mission, Vienna, Austria, 3. 2. 2012
- 4. Prof. Xu Cheng, Dr. A. Class, Karlsruhe Institute of Technology (KIT), Germany, 9. 2. 2012
- Prof. H. M. Prasser, ETH Zürich/Paul Scherrer Institut (PSI), Switzerland, 9. 2. 2012
- Prof. M. Giot, Dr. K. Van Tichelen, SCK CEN/Université Catholique de Louvain, Belgium, 9. 2. 2012
- 7. Dr. U. Hampel, Helmholtz-Zentrum Dresden-Rossendorf, Germany, 9. 2. 2012
- 8. Prof. Y. A. Hassan, Texas A&M University, USA, 9. 2. 2012
- 9. Dr. G. Bandini, Agenzia nazionale per le nuove tecnologie, l'energia e lo sviluppo economico sostenibile (ENEA), Italy, 9. 2. 2012
- Dr. A. Papukchiev, Gesellschaft f
 ür Anlagen- und Reaktorsicherheit (GRS), Germany, 9. 2. 2012
- 11. Dr. F. Perdu, Commissariat à l'Énergie Atomique (CEA), France, 9. 2. 2012
- 12. Dr. R. Schultz, Idaho National. Laboratory, USA, 9. 2. 2012

- Investigation of flow boiling mechanisms in nuclear engineering Slovenian Research Agency Dr. Boštian Končar
- Analyses of ex-vessel molten fuel coolant interaction Slovenian Research Agency Dr. Matjaž Leskovar
- 17. Application and validation of multiscale method for two-phase flow analyses in nuclear reactors
- Slovenian Research Agency Dr. Boštjan Končar
- Simulations of atmosphere stratification breakup experiments with lumped-parameter codes
 - Slovenian Research Agency Asst. Prof. Ivo Kljenak
- Co-financing of the promotion of science Slovenian Research Agency Prof. Leon Cizelj

RESEARCH PROGRAM

- 20. Reactor Engineering
- Prof. Leon Cizelj

R & D GRANTS AND CONTRACTS

- Modelling of material influence on steam explosion Dr. Matjaž Leskovar
- Improvement of safety for existing and new nuclear power plants with probabilistic safety assessment Prof. Marko Tomaž Čepin
- Experiment and simulation of hydrogen combustion in nuclear power plant containment experimental facility Prof. Borut Mayko
- Development of methods and models for simulation of thermal-hydraulic phenomena in innovative nuclear reactors
- Prof. Iztok Tiselj
 Code applications and maintenance program (CAMP); Thermal-hydraulic code applications and maintenance
 Prof. Borut Mavko

NEW CONTRACT

- Expert opinion on Krško NPP tests and repairs during refueling at the end of fuel cycle 25 Milan Vidmar Electroinstitute Ljubo Fabjan, M. Sc.
- 13. A. Shams, Nuclear Research & consultancy Group (NRG), The Netherlands, 9. 2. 2012
- 14. Zhengxiang Chen, University of Manchester, UK, 26. 3.-31. 5. 2012 and 1. 6.-30. 9. 2012
- 15. Youcef Bouaichaoui, Nuclear Research Center of Birine Djelfa, Algeria, 1. 3.-30. 5. 2012
- Dr. Prachai Norajitra, Karlsruhe Institute of Technology (KIT), Germany, 18. 6. 2012
 Edward Spatt de Martipuille, Institut de Padiameteration et de Súpeté Nucléaire (IDON)
- Eduard Scott de Martinville, Institut de Radioprotection et de Sûreté Nucléaire (IRSN), Fontenay-aux-Roses, France, 4. 7. 2012
- Dr. Christine Brun Yaba, Institut de Radioprotection et de Sûreté Nucléaire (IRSN), Fontenay-aux-Roses, France, 4. 7. 2012
- 19. Junghee Hahn, Korea Bussines Center Zagreb, Croatia, 17. 7. 2012
- Dr. HyunKyu Jung, Korea Atomic Energy Research Institute (KAERI), Daejeon, Korea, 17. 7. 2012
- Imre F. Barna, Atomic Energy Research Institute (AEKI), Budapest, Hungary, 27.–31. 8. 2012
 Prof. Hiroshi L. Tanaka, Center for Computational Science, University of Tsukuba,
- Japan, 27. 9. 2012
- Dr. Alexander Bychkov, International Atomic Energy Agency (IAEA), Vienna, Austria, 6. 11. 2012

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- 1. Prof. Leon Cizelj, Head
- 2. Prof. Marko Tomaž Čepin*, left 01.10.12
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- 4. Ljubo Fabjan, M. Sc.
- 5. Asst. Prof. Ivo Kljenak
- 6. Dr. Boštjan Končar
- 7. Dr. Matjaž Leskovar
- 8. Asst. Prof. Marko Matkovič
- 9. Prof. Borut Mavko, retired 28.07.12
- 10. Dr. Andrej Prošek
- 11. Prof. Iztok Tiselj
- 12. Dr. Andrija Volkanovski Postdoctorial associates

13. Dr. Duško Kančev

- 14. Dr. Mihaela Irina Uplaznik
- 15. Dr. Mitja Uršič

Postgraduates

- 16. Ovidiu-Adrian Berar, B. Sc.
- 17. Raphaël Connes, B. Sc.

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18. Oriol Costa Garrido, B. Sc. 19. Martin Draksler, B. Sc 20. Blazhe Gjorgiev, B. Sc. 21. Romain Henry, B. Sc. 22. Tadej Holler, B. Sc. 23. Blaž Mikuž, B. Sc. 24. Jure Oder, B. Sc. 25. Matej Tekavčič, B. Sc. **Technical officers** 26. Sandi Cimerman, B. Sc. 27. Andrej Sušnik, B. Sc. Technical and administrative staff 28. Tanja Klopčič 29. Urška Knific Terze 30. Zoran Petrič, B. Sc. 31. Nataša Pouh, B. Sc.

Note: * part-time JSI member

- Marko Matkovič, Boštjan Končar, "Bubble departure diameter prediction uncertainty", *Sci. Technol. Nucl. Install. (Print)*, vol. 2012, pp. 863190-1-863190-7, 2012.
- 13. Costa Oriol, Iztok Tiselj, Leon Cizelj, "Depressurization of vertical pipe with temperature gradient modeled with WAHA code", *Sci. Technol. Nucl. Install. (Print)*, vol. 2012, pp. 951923-1-951923-9, 2012.
- 14. Andrej Prošek, "RELAP5 Calculations of Bethsy 9.1b Test", *Sci. Technol. Nucl. Install. (Print)*, vol. 2012, pp. 238090-1-238090-11, 2012.
- 15. Andrej Prošek, Ovidiu-Adrian Berar, "Advanced presentation of BETHSY 6.2TC Test results calculated by RELAP5 and TRACE", *Sci. Technol. Nucl. Install. (Print)*, vol. 2012, pp. 812130-1-812130-15, 2012.
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- 21. Jean-Pierre Van Dorsselaere, Ari Auvinen, David Beraha, Patrick Chatelard, Ivo Kljenak, Alexei Miassoedov, Sandro Paci, Th. Walter Tromm, Roland Zeyen, "The European research on severe accidents in generation-II and -III nuclear power plants", *Sci. Technol. Nucl. Install.* (*Print*), vol. 2012, pp. 686945-1-686945-12, 2012.
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PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

(INVITED LECTURE)

- 1. Ovidiu-Adrian Berar, Andrej Prošek, Borut Mavko, "IJS conversion procedure from RELAP5 to TRACE example of achilles test rig", In: *2012 Spring CAMP meeting: May 30-June 1, 2012, Ljubljana, Slovenia*, [S. l., s. n.], 2012, 22 pp.
- 2. Leon Cizelj, "Research and education in nuclear engineering and safety: a national, regional or global activity?", In: *Powerplants 2010: International Conference "Power Plants 2010", 26-29 October 2010, Vrnjačka Banja, Serbia*, [S. l., s. n.], 2010, 10 pp.
- Andrej Prošek, Ovidiu-Adrian Berar, "RELAP5, TRACE 1D and TRACE 3D comparison against Bethsy 9.1b test", In: 2012 Spring CAMP meeting: May 30-June 1, 2012, Ljubljana, Slovenia, [S. l., s. n.], 2012, 17 pp.
- 4. Andrej Prošek, Borut Mavko, Ovidiu-Adrian Berar, "Status of CAMP Activities in Slovenia", In: *Proceedings*, Fall 2012 CAMP Meeeting, November 7-9, 2012, Washington, DC, Washington, U.S.NRC, 2012, 31 pp.

PUBLISHED SCIENTIFIC CONFERENCE CONTRIBUTION

- 1. Ovidiu-Adrian Berar, Andrej Prošek, Borut Mavko, "RELAP5 to TRACE input model conversion procedure and advanced post processing of the results for the ISP-25 test", In: *Proceedings*, 21st International Conference Nuclear Energy for New Europe, Ljubljana 2012, September 5-7, Tomaž Žagar, ed., Samo Fürst, ed., Ljubljana, Nuclear Society of Slovenia, 2012, 12 pp.
- Živa Bricman Rejc, Marko Čepin, "Advanced power system reliability assessment", In: *Proceedings*, 21st International Conference Nuclear Energy for New Europe, Ljubljana 2012, September 5-7, Tomaž Žagar, ed., Samo Fürst, ed., Ljubljana, Nuclear Society of Slovenia, 2012, pp. 1-8.
- 3. Živa Bricman Rejc, Marko Čepin, "Extension of common cause analysis", In: *PSAM11 & ESREL 2012*, 11th International Probabilistic Safety Assessment and Management Conference & The Annual European Safety and Reliability Conference, PSAM11 & ESREL 2012, Helsinki, Finland, 25-29 June 2012, [S. l., s. n.], 2012, pp. 1-10.
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- 6. Leon Cizelj, Daniela Diaconu, Petre Ghitescu, Ivan Ivanov, Iztok Tiselj, Nadja Železnik, "Advancing national and joint nuclear research in the Europena union: the NEWLANCER project", In: *ENS 2012: The European Forum to discuss Nuclear Technology Issues, Opportunities & Challenges, 9-12 December 2012, Manchester, United Kingdom,* Brussels, European Nuclear Society, 2012, 8 pp..
- 7. Leon Cizelj, Daniela Diaconu, Petre Ghitescu, Ivan Ivanov, Iztok Tiselj, Nadja Železnik, "The NEWLANCER project", In: *Proceedings*, 21st International Conference Nuclear Energy for New Europe, Ljubljana 2012, September 5-7, Tomaž Žagar, ed., Samo Fürst, ed., Ljubljana, Nuclear Society of Slovenia, 2012, 9 pp.
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MENTORING

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REACTOR INFRASTRUCTURE CENTRE

RIC

The Reactor Infrastructure Centre incorporates a research reactor TRIGA Mark II Reactor and a Hot Cells Facility. The reactor, operating since 1966, is used for neutron research, training and for producing radioactive isotopes. A detailed technical description of the reactor is available at http://www.rcp.ijs.si/~ric/. The Hot Cells Facility is used for the treatment and handling of radioactive materials and radioactive waste within research and applicative projects. In addition, it is used for performing measurements within the regular radiological monitoring of the reactor.

Besides operating and maintaining the reactor, the members of the reactor staff participate in other activities requiring specialists skilled in the work with sources of radiation and in reactor technology, such as the servicing of industrial radioactive sources and the surveillance of the fuel management in NPP Krško.

In 2012 the reactor operated for 147 days. Altogether, 1307 samples were irradiated in the rotary specimen rack and 37 in the pneumatic transfer system. In addition, 23 pulses were performed. There were no serious operational problems or events influencing nuclear or radiation safety. The reactor operators were performing regular maintenance inspections and activities according to the annual plan.



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tenance inspections and activities according to the annual plan. In the Hot Cells Facility the activities were mostly performed by the Department of Environmental Sciences and the Radiation Protection Unit. The JSI staff performed training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC Enlargement & Integration policy. The treatment and conditioning of low and intermediate radioactive waste for subsequent storage in the central storage for radioactive waste was continuously performed together with the Slovenian Agency for Radioactive waste Management (ARAO). In September, an isotopic thickness gauge was repaired in a single day for Acroni, thus preventing a major

The reactor was mainly operated for the needs of the J. Stefan Institute's Nuclear Training Centre, for educational purposes (Faculty of Mathematics and Physics, University of Ljubljana and Faculty for Energy, University of Maribor) and research departments: the Environmental Sciences, the Reactor Physics and the Experimental Particle Physics.

The reactor was used for the following research:

Reactor physics and neutronics,

economic problem for the company.

- Activation analysis,
- Research on radiation damage of semiconductors,
- Neutron dosimetry and spectrometry,
- Neutron radiography,
- Activation of materials, nuclear waste and decommissioning,
- Irradiation of materials for fusion reactors,
- Irradiation of electronic and medical components,
- Development and testing of new detectors,
- Development of new methods for measuring power profiles, neutron spectra, etc.,
- Verification and validation of methods for calculating the transport of neutrons, photons and electrons,
- Development of educational tools in reactor physics.

The TRIGA reactor participates in the FP7 AIDA (Advanced Infrastructures for Detectors and Accelerators) project that brings together advanced European infrastructures for future particle-physics experiments.

Within the collaboration with CEA irradiation related to two projects, led by the Reactor Physics Division, were conducted. In the frame of "Analysis of thermal power calibration method and joint experimental irradiation campaign at TRIGA research reactor" accurate in-core flux mapping measurements were performed and various SPND- and SPGD-type detectors tested. Within the frame of the "Experimental Verification of Kinetic Parameters of the TRIGA Reactor and the Upgrade of the Digital Meter of Reactivity" everything for the experimental campaign in May 2013 was prepared.

In September 2012, a contract was signed for the irradiation and testing of electronic instruments with National instruments and the ITER organization. The project was entitled Thermal neutron irradiation testing of NI PXI and cRIO products.

At the end of 2012 a collaboration with INMEDICA, Slovenian Device Incubator for Medical Systems and Treatments, was established, in frame of which medical equipment is irradiated and the changes after irradiation are observed.



Figure 1: Air bubbles produced during the void reactivity coefficient measurements.

Together with the Nuclear Training Centre and NPP Krško the project for modernizing practical exercise on the TRIGA reactor was brought up. Some new experimental equipment was acquired and new software developed for connecting all the hardware and to perform the exercises.

Practical exercises in reactor physics and kinetics for the students of physics at the University of Ljubljana were performed. Some of the exercises were performed for the first time in the history of the reactor.

The work on the Periodic Safety Report that started in 2011 was continued.

The reactor operators took part in the outage of NPP Krško.

Before the reactor start-up at the NPP Krško preparations and tests to conduct physical tests took place at the TRIGA reactor.

The project within the framework of IAEA Technical Coordination Programme entitled "Carrying out a Feasibility Study and Installing the Thermal

Neutron Driven 14 MeV Neutron Converter into the TRIGA Research Reactor" was continued.

The reactor operators supported the researchers by performing the operations and services for which the researchers are not qualified and authorized, such as operating the reactor, performing irradiations and manipulating radioactive samples.

The research results were published in approximately 20 scientific papers. Seven young researchers performed their research at the reactor.

In November 2012 an IAEA INSARR mission was conducted. The objectives of the mission was to review the operational safety of the reactor, including reactor management and regulatory supervision, Safety Analysis Report, safety analyses, Operational Limits and Conditions, conduct of operations, maintenance, training and qualifications of operating personnel, utilization and modifications, operational radiation protection and waste management, emergency planning, quality assurance and decommissioning plan. The mission was conducted in accordance with the IAEA procedures by a team composed of IAEA experts from Argentina, France, Israel and Morocco.

In 2012 the following international courses in the field of safety of research reactors were performed:

- IAEERRI12: IAEA Group Fellowship Training, Programme on Research Reactors, 1. 10. 2012–12. 10. 2012, 10 participants
- 2. TJET13: Nuclear Power Plant Technology, ICJT,7. 11. 2012-2. 4. 2012, 15 participants
- 3. TJET14: Nuclear Power Plant Technology, ICJT, 7. 11. 2012-5. 4. 2013, 22 participants

Practical exercises in reactor physics and kinetics for students of physics at the University of Ljubljana were performed. The post-graduate students of nuclear engineering attended some of these exercises as well. For these purposes the reactor operated approximately 2 months. The reactor was also used for practical exercises within the training program of the NPP Krško reactor operators. The exercises were prepared and carried out by the reactor personnel in cooperation with the Nuclear Training Centre and the Department of Reactor Physics.

In 2012, there were more than 50 short group visits to the reactor. The visitors were mainly foreign scientists, students and more than 33 groups of school children. The total number exceeded 900.

INTERNATIONAL PROJECTS

- 1. Reports on thermal neutron induced SEU susceptibility of PXIe and cRIO fast controller components
 - ITER Organization

Dr. Luka Snoj

- Training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC enlargement and integration policy Institute For Reference Materials And Measurements Prof. Borut Smodiš
- Training fee for Ms Gulnura Abasova (Kyrgyzstan), TA00221759, 2. 2.–1. 5. 2012 Ictp/iaea Step Program, The Abdus Salam Prof. Peter Stegnar
- Training fee for Ms Ilona Matveyeva (Kazakhstan), TA00221835, 15. 2.–14. 5. 2012 Ictp/iaea Step Program, The Abdus Salam Prof. Peter Stegnar
- NATO SPS.EAP.SFP 984524: Radioactive and heavy metal waste tailings risk reduction in Fergama Valley, Kyrgyz Republic

NATO Prof. Peter Stegnar

- IAEA Fellowship for Mr Dieudonne Gelembo Kom'Bele, C6/ZAI/11002 IAEA - International Atomic Energy Agency Prof. Borut Smodiš
- Automation of a pneumatic transport system for neutron activation analysis IAEA - International Atomic Energy Agency Prof. Borut Smodiš
- IAEA Fellowship for Mr Bouzekri Nacir and Mr Moussa Bounakhla (MOR/12014V, MOR/12015V)

IAEA - International Atomic Energy Agency

Prof. Borut Smodiš 9. Training fee for Ms Ilona Matveyeva (Kazakhstan), 24. 9.-23. 12. 2012 ICTP - Centro Internazionale Di Fisica Teorica Prof. Borut Smodiš

R & D GRANTS AND CONTRACTS

- 1. Calculations to support neutron monitor calibration JET fusion reactor example case Dr. Luka Snoj
- 2. Lease and usage of the hot cell. Prof. Borut Smodiš

NEW CONTRACTS

 Treatment and conditioning of radioactive waste for storage ARAO Prof. Borut Smodiš

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- 2. Expert opinion in Krško NPP tests and repairs during refueling at the end of fuel cycle
- Expert opinion in Krško NPP tests and repairs during refueling at the end of fuel cycle 25

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CENTRE FOR NETWORKING INFRASTRUCTURE

CNI

The basic function of the Centre for Networking Infrastructure (CNI) is the management and maintenance of the JSI computer network, including planning, development, upgrades, maintaining contact with public networks, and providing security. The CNI also houses and supports the local SiGNET GRID cluster.

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Figure 1: JSI connectivity structure

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Figure 2: Layout of JSI communication network *Photo by Sašo Rebolj Playboy

SCIENCE INFORMATION CENTRE

SIC

The Jožef Stefan Institute Science Information Centre is the central Slovenian physics library and one of the largest special libraries in Slovenia. Our main tasks are the acquisition, archiving, and loan of books and periodicals, and the input, update and control of bibliographic data of the Institute staff, as requested by the funding ministry.

Our collection covers the fields of physics, chemistry, biochemistry, electronics, information science, artificial intelligence, nuclear technology, energy management and environmental science. We are a full member of the Slovenian library cooperative, COBISS, and use their services to catalogue and loan our materials. You can check what is new in the library, browse our online catalogue, or send inter-library loan requests using our WWW site.

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We manage a bibliographic database of the Institute's production. The database contains about 80,000 records, Dr. Luka Šušteršič going back to the Institute's inception in 1949. The records of last year's work are included as part of this report.

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- Jože Škulj
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- Slavka Šmuc, B. Sc., retired 31.12.12
- 10. Branka Štrancar 11. Nada Tratnik
- 12. Saša Žnidar

ENERGY EFFICIENCY CENTRE

EEC

The basic activities of the Energy Efficiency Centre are in efficient energy use, long-term planning in energy and the reduction of greenhouse-gases emissions. The centre is a focal point for the collection and transfer of energy-efficiency technologies to energy users, the state, energy service and equipment providers, and other interested agencies. At the same time it covers the environmental effects of energy use and conversion. The most significant part of the EEC's activities is thus cooperation with state institutions in the preparation of strategic documents and legislation in the field of efficient energy use, energy planning, distributed electricity production, emission trading; nevertheless, it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as being more and more involved in European research projects.



Energy and the environment

In 2012 the Energy Efficiency Centre with its professional work ensured a quality support to ministries in the Head: preparation of development strategic documents and the transfer of EU legislation in the field of energy planning, Stane Merše, M. Sc. energy efficiency, use of renewables and greenhouse-gases emissions reduction.

The accepted EU climate-energy package set new and ambitious goals for Slovenia regarding an increase of energy efficiency, the exploitation of renewables and the reduction of greenhouse-gases emissions. Efficient

energy use is a priority field for achieving these goals, in accordance with the requirements of the European Commission and the new directive on energy efficiency (2012/27/EU). The preparation of evaluation methodologies for performing energy-efficiency measures, which represent a key tool in presenting the fulfilment of set goals, was going on.

For the Energy Agency an integrated analysis and a report on achieving national goals in the field of renewables and cogeneration for the period 2010-2011 was elaborated.

The center cooperates with the Statistical Office of the Republic of Slovenia, where it prepares a model calculation of fuels and energy use in households for the national energy statistics.

The R&D work of the Energy Efficiency Centre is an important contribution to the preparation of support to industry it significantly contributes to an increase of competitiveness and development

Also in 2012, the center continued with activities of the state referential centre for energy by the preparation of a set of indicators for energy and the environment, as well cooperating in the carrying out of the research of energy efficiency in households REUS.

In the field of GHG emissions reduction, the centre prepared for the Ministry of Agriculture and Environment new projections of GHG and air pollutants' emissions from the NEC directive by the year 2030, a report for the European

Commission and framework projections of emissions by the year 2050. It also cooperated in the preparation of strategic studies for determining the goals of RS in the revised Göteborg Protocol.

In 2012 the successful cooperation with the Municipality Ljubljana (MOL) continued, where the center harmonized with the EIB an elaborated investment programme of the energy renovation of public buildings owned by the MOL and the application for technical help ELENA. At the end of the year the municipality signed a contract with EIB on subsidizing technical help ELENA to the amount of €1.35m, which will enable the preparation of projects for carrying out the energy renovation of units to the amount of €50m using a model of energy contracting.

Promotion of efficient energy use and energy consulting

The Energy Efficiency Centre in 2012 continued with its training activities where the fifth cycle of energy managers training was successfully concluded within the European programme EUREM. In the autumn, the Figure 1: Development of distributed electricity production - role of sixth cycle of training already started. Due to the very positive reaction of the cogeneration in ensuring peak electricity needs in winter time

key documents in Slovenia in the field of energy development, energy efficiency, renewables exploitation and the transition of Slovenia to a low-carbon society, with training activities and restructuring.





Figure 2: New installed measurement and communication equipment for monitoring electricity use in RCP JSI premises

participants and their interest (in Slovenia there is already more than 120 energy managers with a EUREM licence), it is clear that there is a great need for such training. High-quality knowledge in this field is of key importance for the execution of efficient solutions in practice.

In 2012 the Center of Energy Efficiency carried out several consulting tasks in industry and performed a series of energy audits for enterprises and institutions to reduce the consumption and costs for energy and emissions. Among the larger clients were Luka Koper, Thermo Power Plant Ljubljana, Borzen – Support Center, BTC, Telekom Slovenia.

The center professionally cooperated with the company Petrol d.d. in carrying out the biggest programme of large consumers for ensuring the energy savings of end users and for the company Elektro Gorenjska Prodaja d.o.o. we prepared a programme for the energy efficiency of households.

The centre also prepared the programme and cooperated in the fourteenth execution of the largest Slovenian conference of energy managers "Energy Managers Days", the annual meeting of energy managers, with more than 200 participants confirms the quality and the public profile of the EEC's professional work.

International cooperation

In 2012 the EEC carried out as many as 12 international projects, financed from the European Union resources in the framework of the 7th Framework Programme and the European Commission programme "Intelligent Energy for Europe" as well as MEDITERAN and South East Europe.

Projects cover activities in the fields of:

- development of innovative systems of energy use monitoring and management in industry (Life Saver, 7th FP),
- advanced intelligent systems for energy management in the cities (ISEMIC),
- increase of the energy efficiency of existing non-residential buildings with the introduction of the costeffective optimization of energy systems Re-Commissioning (Re-Co),
- analysis of the impacts of the introduction of smart energy measurements on the use and costs of energy in low-income housing (Elih-MED),
- inclusion of criteria of energy efficiency in public tenders (EFFECT),
- promotion and development of new energy services (ChangeBest),
- development and carrying out of energy contracting and advanced energy services (EESI),
- compiling and elaboration of current data on renewable energy sources use (EurObserv`ER Barometer),
- monitoring and promotion of cogeneration development (CODE2),
- carrying out the EU directive on energy services and evaluation energy efficiency measures (CA ESD),
- carrying out the EU directive on renewable energy sources (CA RES),
- monitoring of indicators of energy use and energy efficiency in EU (ODYSSEE MURE EU-27).



Figure 3: Monitoring of hourly water consumption at the Reactor Centre Podgorica

The projects include cooperation with R&D organisations from Europe with a strong emphasis on concrete applications and the promotion of energy efficiency. In the framework of each project the EEC staff took part in numerous foreign professional meetings and visits.

The center is included in intensive research work in the field of intelligent energy management in industry within the projects LifeSaver and ISEMIC. One of the results is also the installation of the first part of the electricity and water management system at the Reactor Centre JSI in Podgorica.

Some outstanding achievements in 2012

1. Preparation of several key support documents for the government of the Republic of Slovenia in the field of energy policy (Green paper and strategic studies for the National Energy Programme), energy efficiency (First and Second National Action Plan for Energy Efficiency), renewable energy sources (Action Plan for Renewable energy sources for the period 2010–2020) and climate policy (Operative programme of GHG emissions reduction up to 2012).

- Establishment of energy managers training in the framework of the European project EUREM and 2. professional support to industry and other institutions by carrying out energy audits, feasibility studies and other consulting (Goodyear, TE-TOL, Cinkarna Celje, Litostroj, TE-TOL, Luka Koper etc.).
- 3. Cooperation in different international projects in the framework of European Commission programmes in the fields of energy efficiency, energy management, combined production of electricity and heat, promotion of energy efficient technologies and energy services, exploitation of wood biomass and others

Organization of conferences, congresses and meetings

- Energy Managers Days 2012 14th Meeting of Energy Managers of Slovenia, Portorož, 16.- 17.4.2012 1
- European Energy Manager Training, Ljubljana, 18.1.-20.1., 14.3.-16.3., 9.5.-11.5. in 15.6.2012 2.
- Workshop on the project EESI and ChangeBest and EESI Services of EEU in practice, Ljubljana, 23.5.2012. 3.

INTERNATIONAL PROJECTS

- 1. 7. FP . LifeSaver: Context sensitive monitoring of energy consumption to support energy savings and emission trading in industry European Commission
- Boris Sučić, M. Sc.
- 2. Good practice examples of changes in energy service business, strategies and supportive policies and measures in the course of the implementation of directive 2006/32/EC; ChangeBest; IEE/08/434/SI2.528383 European Commission
 - Barbara Petelin Visočnik, M. Sc.
- EESI European energy service initiative; IEE/08/581/SI2.528408 3. European Commission
- Damir Staničić, M. Sc.
- 4. IEE EurObservER2020: The EurObserv'ER barometer backs the new RES directive European Commission Dr. Fouad Al-Mansour
- EIE ODYSSEE MURE 2010: Monitoring of EU and national energy efficiency targets, 5. IEE/09/801/SI2.558254 European Commission
 - Dr. Fouad Al-Mansour
- 6. ELIH-Med Energy efficiency in low-income housing in the Mediterranean Joint Technical Secretariat Med Programme
- Aleš Podgornik, M. Sc. EFFECT - Upgrading of energy efficient public procurement for a balanced economic growth of SEE area
 - Agenzia Regionale Per L'Energia
 - Polona Lah, B. Sc.
- 8 Re-Co: Re-commissioning-raising energy performance in existing non-residential buildings
 - European Commission
 - Barbara Petelin Visočnik, M. Sc.
- EIE C.O.D.E. 2: Cogeneration observatory and dissemination Europe 2; IEE/11/910/ SI2.615940 European Commission
 - Stane Merše, M. Sc.
- 10. CEEM Central environmental and energy management as a kit for survival European Commission Matevž Pušnik, M. Sc
- 11. EIE C.O.D.E: Cogeneration observatory and dissemination Europe; IEE/07/564/ SI2.499462
 - Cogen Europe
 - Stane Merše, M. Sc.
- 12. SEE-ERA.NET PLUS ISEMIC: Intelligent information system for monitoring and verification of energy management in cities University of Zagreb Boris Sučić, M. Sc.

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13. Organization of a study visit on the theme of energy statistics and energy efficiency Adetef Assistance Technique France Dr. Fouad Al-Mansour

RESEARCH PROGRAM

Modelling and environmental impact assessment of processes and energy technologies 1 Dr. Fouad Al-Mansour

R & D GRANTS AND CONTRACTS

- Environmental footprint of agriculture and food processing industry and technological measures for its lowering in the future Dr. Fouad Al-Mansour
- 2. EIE- EUREM.NET: Training and network of european energy managers, N 112/06; EUREM I-VI Stane Merše, M. Sc.
- Preparation of a lecture competition of Slovenian communities in energy efficiency and 3. renewables Boris Sučić, M. Sc.

NEW CONTRACTS

- Professional cooperation in the web application "Energy consultant modules: transport, electricity and heating / cooling Informa Echo, d. o. o. Marko Pečkaj, B. Sc.
- Carrying out of the project Concerted actions in the field of the Directive on end energy use efficiency (CA ESD II)
- Ministry of Infrastructure and Spatial Planning Damir Staničić, M. Sc. 3
- Energy efficiency obligation scheme for large energy sales companies Petrol d. d., Ljubljana Damir Staničić, M. Sc.
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- Cladia di Benedetto, Friuli Innovazione, Udine, Italy, 7.12.12
 Romina Kocina, Friuli Innovazione, Udine, Italy, 7.12.12
- 10. Polona Lah, B. Sc.
- 11. Marko Pečkaj, B. Sc.
- 12. Barbara Petelin Visočnik, M. Sc.
- 13. Aleš Podgornik, M. Sc.
- 14. Boris Sučić, M. Sc.

Technical and administrative staff

15. Roza Pergarec, B. Sc.

16. Igor Ribič

Note:

- ** postgraduate financed by industry
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PROFESSIONAL MONOGRAPH

1. Fouad Al-Mansour, Matjaž Česen, Energy efficiency policies and measures in Slovenia in 2012: ODYSSEE-MURE 2010, Monitoring of EU and national energy efficiency targets, Ljubljana, Intelligent Energy Europe, 2012.

MENTORING

1. Matevž Pušnik, *Integrated resource planning and national energy systems modelling:* master's thesis, Ljubljana, 2012 (mentor Andrej Gubina).

CENTRE FOR ELECTRON MICROSCOPY

CEM

The Centre for Electron Microscopy (CEM) has the function of a supporting infrastructure center at the JSI. It comprises the equipment for electron microscopy that is necessary for the research work of the departments K5, K6, K7, K8 and K9. Other JSI departments, research institutes, universities and industry also have access to the equipment. The users of the CEM equipment are the researchers in the field of materials science that are involved in the chemical and structural analyses of materials on the micro and atomic scales. The major equipment of the CEM represents two scanning electron microscopes (JSM-840A and JSM-5800) and two transmission electron microscopes (JEM-2000FX and JEM-2010F). CEM coworkers also manage the transmission electron microscope JEM-2100, which belongs to the Center of Excellence NiN, and in 2009 the newly installed field-emission scanning electron microscope JSM-7600F, which was a joint purchase by ten JSI departments and also the faculties NTF and FKKT of the University Ljubljana. In 2010 the electron microscopes were upgraded with the following analytical attachments that were purchased by the Excellence Centre NAMASTE: CCD camera on the JEM-2010F, ADF detector on the JEM-2010F and EBSD system on the JSM-7600F.



Prof. Miran Čeh

Scanning electron microscopy (SEM) is used for morphological studies of either fractured or polished surfaces. Since both scanning electron microscopes are equipped with X-ray spectroscopy (EDXS, WDXS), qualitative and quantitative chemical analyses on the micro scale are also possible. Since only a few µm³ of the material are non-destructively analyzed, the term electron-probe microanalysis (EPMA) is used for such analytical work. Apart from EDXS and WDXS, the new FEG-SEM JSM-7600F is also equipped with electron lithography.

When the structural features on the nanoscale are investigated, however, the various techniques of transmission electron microscopy (TEM) are used. In particular, the JEM-2010F is a state-of-the-art TEM/STEM microscope with a FEG (field-emission gun) electron source and a point-to-point resolution below 0.19 nm, which is more than sufficient to observe the atomic columns in crystalline materials. The JEM-2010F is also equipped with an annular dark-field detector (HAADF-STEM) for so-called Z-contrast imaging, which enables the chemical analysis of a single atomic column on the basis of the measured intensities. Both transmission electron microscopes are additionally equipped with analytical systems for chemical analysis (EDS, EELS). The CEM also comprises the equipment for SEM and TEM specimen preparation, which is the starting point for all electron-microscopy observation procedures. Especially important are the high- and low-energy ion-millers, which enable the preparation of thin foils that are transparent to high-energy electrons.

The analytical work that is performed on the CEM equipment varies in terms of both the investigated materials and/or the used electron microscopy techniques. While scanning electron microscopy is used mainly for the microstructural characterization and chemical analysis of polycrystalline ceramic materials (functional ceramics, engineering ceramics, bio-ceramics, and composites), magnetic materials, glasses, metals, alloys, etc., transmission electron microscopy is used for structural and chemical investigations of grain boundaries, planar faults, dislocations and precipitates within the same materials. The structural and chemical analysis of grain boundaries is especially important since it is known that the physical properties to a great extent depend on the structure and chemistry of grain boundaries.

In order to be able to perform electron microscopy investigations it is imperative that the equipment in the CEM is well maintained. In view of this,



Figure 1: TEM-BF image of antiphase boundaries in a grain of 760°C-sintered BiFeO₃ ceramics in the [01-1] zone axis. The marked diffraction spot on the SAED pattern corresponds to the set of spots in the $(\sqrt{2}, \sqrt{2}, \sqrt{2})$ positions, which are due to oxygen shifts in the octahedrally tilted BiFeO3 structure.

Electronic Ceramics Department: T. Rojac, A. Benčan, G. Dražić, M. Kosec, D. Damjanović, Piezoelectric nonlinearity and frequency dispersion of the direct piezoelectric response of BiFeO3 ceramics. J. Appl. Phys., 2012, vol. 112, no. 6, pp. 064114-1-064114-12

one on the main tasks is to attain the maximum possible operational time for the microscopes. This complex and expensive equipment needs regular daily maintenance, apart from the servicing. Other activities of the CEM are the organization of the training courses for operators and the implementation of new analytical methods, which is realized with the help of CEM co-workers.



Figure 2: The β -3-calcium phosphate crystals on the surface of a zirconia ceramic substrate.

Engineering Ceramics Department: M. Štefanič



Figure 3: Aggregate of colour-pigment microcapsules. Department fo Nanostructured Materials: Z. Samardžija



Figure 4: High-resolution transmission electron microscopy (HREM) image of a nanocomposite particle containing a thin $BaFe_{12}O_{19}$ hexaferrite (HF) layer intergrown into a spinel (S) iron-oxide matrix of γ -Fe₂ O_3

Department for Materials Synthesis: D. Primc



Figure 5: TiO_2/Au composite with inverse opal structure: the composite is a novel material with specific structural properties that benefits its surface and optical properties. The uniform 3D porosity of the material increases its surface contact area. The structure contributes to the specific optical properties as a consequence of the combination of: (i) the SRP of Au metallic nanoparticles in contact with a TiO_2 semiconductor and (ii) the photonic bandgap properties of the optical crystal. The material has the potential for applications in various separation processes, catalysis, photonic bandgap materials and innovative emerging biomedical nanotechnologies.

Department for Advanced Materials: M. Vukomanović

STAFF

Researchers 1. Prof. Miran Čeh, Head Technical and administrative staff

2. Hamdija Hodžić, B. Sc.

CENTRE FOR KNOWLEDGE TRANSFER IN INFORMATION TECHNOLOGIES CT-3

The Centre for Knowledge Transfer in Information Technologies performs educational, promotional and infrastructural activities and provides for the direct exchange of information and experience between researchers and the users of their research results.

By partnering and active engagement in different European research projects the centre successfully extends its activities to research and development. Most of the research is performed in the area of knowledge management for traditional and emerging forms of organizations, like networked and virtual organizations. In 2012 the centre was active in several European projects from FP7: PASCAL2 (Pattern Analysis, Statistical Modelling and Computational Learning 2), METANET (Multilingual Europe: a Technology Alliance), ENVISION (ENVIronmental Services Infrastructure with Ontologies), GENDERA (Gender Debate in the European Research Area), RENDER (Reflecting Knowledge Diversity), ALERT (Active support and Real-time Coordination based on Event Processing in Open Source Software Development), PLANETDATA (A European Network of Excellence on Large-Scale Data Management, e-LICO (An e-Laboratory for Interdisciplinary Collaborative Research in Data Mining and Data-Intensive Science), Head: TRANSLECTURES (Transcription and Translation of Video Lectures), X-LIKE (Crosslingual Knowledge Extraction), Mitja Jermol, M. Sc. MOBIS (Personalized Mobility Service for energy Efficiency and Security through Advanced), MEDIAMIXER (Com-

munity Set-up and Networking for the Remixing of Online Media Fragments), NRG4CAST (Energy Forecasting), SOPHOCLES (Self-Organised information Processing, Criticality and Emergence in multile), CENTRAL COMMUNITY (Emerging communities for collective innovation in Central Europe).

In 2012 the Centre for Knowledge Transfer in IT was actively involved in 15 European projects.

In 2012 the centre was active in 15 European projects. The centre prepares and organizes carefully designed educational events, such as: conferences, seminars, workshops, and summer schools. They are targeted at experts who would like to apply the latest knowledge and achievements from intelligent data analysis, knowledge technologies, data mining, text mining and decision support to the areas of network organizations, business decisions, finance, marketing, automation and process control. A special consideration is put on the managers and decision makers who are aware of the strengths and benefits to the success of their business.

All educational events are designed to transfer basic, additional and latest expert knowledge to the companies, research and educational organizations. In order to make the knowledge transfer efficient we are combining traditional and ICT-supported training methods. For this purpose we are operating a number of training web portals. The most popular one is http:// videolectures.net/. It now offers more than 16,300 recorded tutorials from different scientific events and is visited every month by an average of 175,000 visitors from around the world. The main purpose of the portal is to provide free and open access to high-quality video lectures presented by distinguished

CT3 is operating two web portals. The first one is http://videolectures.net/, which is now becoming a reference portal presenting highquality scientific lectures and the second one is http://www.ist-world.org, which offers services for automatic data collection and an analysis of European research.

scholars and scientists at the most important and prominent events. In today's world VideoLectures.NET presents a free knowledge hub, a way of opening up education to everyone for everyone and as there is a great need to share educational content on all levels in order to benefit society and foster economy. It also gives a learning opportunity to audiences of all social levels.

We have successfully collaborated within the Videolectures.net portal with some of the top ten American Universities MIT (Massachusetts Institute of Technology), University of California - Berkeley, YALE, John Hopkins University, University of California, Irvine, and Carnegie Ethics Studio, as well as with the European CERN and ETH from Zurich. VideoLectures.Net has strong connections in OpenCast Foundation, OpenCourseWare Consortium and Knowledge 4 All Foundation Ltd.

The centre also operates a web portal http://www.ist-world.org that offers services for automatic data collection and an analysis of European research. The user can perform several simple and complex analyses, predictions and detect trends in research. The database currently contains data about 100,000 research organizations, 42,500 research projects and around

The portal http://videolectures.net/ collaborates with the Massachusetts Institute of Technology (MIT), YALE, University of California - Berkeley, Universities of Ljubljana and Maribor, and with European Organization for Nuclear Research - CERN. VideoLectures.Net has strong connections in the OpenCast Foundation, **OpenCourseWare Consortium and Knowledge 4** All Foundation Ltd.

2 million experts from Europe. This is an exceptional web service that is being visited every day by an average of 5,000 unique visitors.

In 2012 we organized the 7th Student Competition in Computer Science, attended by 172 students from Slovenian secondary schools and a video competition, attended by 104 students. We have also organized project meetings for different EU projects (RENDER and TRANSLECTURES) and an international workshop for the EU project TRANS-LECTURES "Workshop on Co-creation of emerging trends in Academia", which was attended by 69 experts. We also organised in collaboration with the Slovenian Chamber of Commerce and Industry and Slovenian Technology Agency, a one-day workshop "Preparing a competitive project proposal for FP7 calls in 2013". At the 15th international Information Society - IS 2012 multiconference we organised a FORSEE - Technological Forecasting in ICT workshop.

Our role in the FP7 integrated projects XLike "Cross-lingual Knowledge Extraction" in RENDER - Reflecting Knowledge Diversity and in three networks of excellence PASCAL2, PLANETDATA and META-NET was the support and coordination of all educational and dissemination activities as well as knowledge transfer.

Organization of conferences, congresses and meetings

- 7th Student competition in computer science, Ljubljana, 24. 3. 2012 1.
- 2. Project meeting of the EU project RENDER, Dubrovnik, Croatia, 5.–6. 7. 2012
- Meeting of the Harvest group inside of the EU project PASCAL, 9.-13. 7. 2012 3.
- 4. National Open Consultation Event at the 15th international Information Society - IS 2012, 10. 10. 2012
- 5. Workshop "Preparation of project proposal for FP7 2013", Ljubljana, 5. 11. 2012
- Workshop on co-creation of emerging trends in Academia, Ljubljana, 7. 11. 2012 6.
- Project meeting of the EU project transLectures, Ljubljana, 8.-9. 11. 2012 7.
- 8. Workshop "Advance use of modern information technologies to fight corruption" at the conference EPAC, Barcelona, Spain, 22. 11. 2012

INTERNATIONAL PROJECTS

1. 7. FP - EURIDICE: European inter-disciplinary research on intelligent cargo for eficient, safe and environment-friendly logistics European Commission

Mitja Jermol, M. Sc.

- 7. FP PASCAL2: Pattern analysis, statistical modelling and computational learning 2 2 European Commission Mitja Jermol, M. Sc.
- 3. 7. FP - COSMOS: Cooperation of space NCPs as a means to optimise services European Commission
- Dr. Špela Stres 4. 7. FP - GENDERA: Gender debate in the European research area European Commission
- Mitja Jermol, M. Sc.
- 7. FP ENVISION: Environmental services infrastructures with ontologies 5. European Commission Mitja Jermol, M. Sc.
- FP MetaNET: Technologies for the multilingual european information society 6. European Commission
- Mitja Jermol, M. Sc. 7.
- FP RENDER: Reflecting knowledge diversity European Commission
- Mitja Jermol, M. Sc. 8. FP - PlanetData
- European Commission Mitja Jermol, M. Sc.
- 7. FP ALERT: Active support and real-time coordination based on event processing in 9. open source Software Development European Commission
 - Mitia Iermol. M. Sc.
- 10. 7. FP - e-LICO: e-Laboratory for collaborative interdisciplinary research in data ining and data intensive sciences

VISITORS FROM ABROAD

- 1. Manan Vohra, Digital Consultant London, Great Britain, 8.-11. 7. 2012
- Joan Albert Silvestre Cerda, UPVLC, Spain, 9. 7.-9. 10. 2012 Alfons Juan, UPVLC, Spain, 9.-13. 7. 2012 2.
- 3.
- 4 Colin de la Higuera, Nantes University, France, 9.-13. 7. 2012
- Sandeep Manchella, India, 3. 8.-27. 10. 2012 5.
- Abraham B. Hsuan, Irwin & Hsuan LLP, USA, 5.-9. 11. 2012 6.
- 7 Ramesh Viswanathan, Siemens Corporate Research, USA, 6, -7, 11, 2012

European Commission Mitja Jermol, M. Sc.

- 7. FP transLectures: Transcription and translation of video lectures 11 European Commission
- Mitja Jermol, M. Sc
- 12. 7. FP MEDIAMIXER: Community set-up and networking for the remixing of online media fragments European Commission
- Mitja Jermol, M. Sc.
- 13. 7. FP MobiS: Personalized mobility services for energy efficiency and security through advanced artificial intelligence techniques European Commission

Mitja Jermol, M. Sc.

- 14. 7. FP X-Like: Cross-lingual knowledge extraction European Commission
 - Mitia Iermol. M. Sc.
- 15. 7. FP Sophocles: Self-organised information processing, criticality and emergence in multilevel systems European Commission

Marjana Plukavec, B. Sc.

- 16. 7. FP NRG4CAST: Energy forecasting European Commission Mitja Jermol, M. Sc.
- CE Central community-emerging communities for collective innovation in Central Europe European Commission Mitja Jermol, M. Sc.

R & D GRANTS AND CONTRACTS

- CC CLASS: Cloud Assisted Services 1
- Mitja Jermol, M. Sc. 2. National open consultation event - ICT Foresight exercise
- Špela Sitar, B. Sc.
- 8. Colin de la Higuera, Nantes University, France, 5.-8. 11. 2012
- Olaf Schulte, ETH Zurich in Opencast Matterhorn, Switzerlan, 6.-9. 11. 2012
- 10. Meena Hwang, OpenCourseWareConsortium, USA, 6.-10. 11. 2012
- 11. John Shawe-Taylor, University College London, Great Britain, 6.-8. 11. 2012
- 12. Clive P.L. Young, University College London, Great Britain, 6.-8. 11. 2012
- 13. Abel Caine, Unesco, France, 6.-8. 11. 2012
STAFF

Technical officers Mitja Jermol, M. Sc., Head Davor Orlić, B. Sc. Marjana Plukavec, B. Sc. Špela Sitar, B. Sc.

Tanja Zdolšek, B. Sc.
 Technical and administrative staff
 Ana Fabjan
 Adis Krečo, B. Sc.
 Monika Kropej, B. Sc.

MILAN ČOPIČ NUCLEAR TRAINING CENTRE ICJT

The mission of our training centre is training in the field of nuclear technologies and radiation protection. In addition we are actively informing the public about those technologies.

Training in the area of nuclear technologies is our primary mission. In recent years there has been a change of generations in NPP Krško; consequently, for the fifth calendar year in a row we have been conducting two *Nuclear Technology* courses, which are the initial theoretical training for future control-room operators. The first such course started in the autumn of 2011 and ended in the spring of 2012, and the second started in the autumn of 2012 and will end in the spring of 2013. Furthermore, there was a course *Basics of Nuclear Technology*, which is intended for non-control-room personnel of NPP and participants from other organizations. At the request of the company Numip we have also developed the program of a new, one-week course *Fundamentals of Nuclear Technology*, which was subsequently conducted at their premises for the staff of Numip and a course "Use of programs for core analysis (LOADF, SHUFFLE in INCORE-3D)", intended for the staff of NPP Krško.



Prof. Igor Jenčič

There were 17 radiological protection training courses for the medical, industrial and research use of radioac-

We have conducted 8 international courses, among those 5 radiochemistry courses financed by the EU for the participants from accession countries and where the lecturers were researchers from the Environmental Sciences Department (O2). The EU has, through the ITER consortium, also funded a course for the staff of regulatory bodies of third countries, where the bulk of lectures were given by experts from the Reactor Engineering Division (R4).

Due to the generation change in NPP Krško the training in the area of nuclear technologies at the Nuclear Training Centre has been very intensive for the fifth year in a row.

A course of reactor physics by the use of research reactors – EERRI, financed by the IAEA, was already the fourth such course. The lecturers at this course were Nuclear Training Center, Reactor Physics Division (F8), Reactor Infrastructure Centre (RIC) and the Radiation Protection Unit (SVPIS). The course GTRI, organized by the U.S. National Nuclear Security Agency, had a one-day practical exercise on our premises.

Public information remains a very important part of our activities. Groups of visitors (mainly schoolchildren, students and various societies) were regularly attending lectures on electricity from nuclear energy, on radioactive waste, and about fusion. They have also visited the permanent exhibition on nuclear energy. Altogether, there were 164 groups or 7264 visitors this year. Since 1993 our information centre has been visited by a total of 142680 pupils, teachers and other visitors. We have continued monitoring and analysing media reports on nuclear energy. An important part of the information activity is the *Fusion Expo* project, which is funded by the European Fusion Development Agreement. The travelling exhibition on fusion – in some locations parts of it – has been set up in Nancy and Aix-en-Provence (France), Charleroi and Liege (Belgium), Ljubljana (Slovenia), Karlsruhe (Germany), as well as in Rome and Genova (Italy).



Figure 1: Deputy Director General, dr. Alexander Bychkov addressed the trainees of the Nuclear Technology course during his visit to the JSI Reactor Centre on November 6, 2012.



Figure 2: The Open day of the JSI attracted many young visitors to the Nuclear Training Centre.

	Table of training activities at Nuclear Training Centre in 2012				
Date	Title of the course	Participants	Lecturers	Weeks	Participants × Weeks
(7.11.2011) - 30.3.	Nuclear Technology, Theory	15	21	14	210
9.1 16.1.	Radiation protection for RP department staff - refresher course	13	3	0.8	10.4
20.2 22.2.	Radiation protection for industrial and other practices (unsealed sources)	6	5	0.6	3.6
20.2 7.3.	Radiation protection for industrial and other practices (radiography)	2	4	0.8	1.6
20.2 22.2.	Radiation protection for industrial and other practices (sealed sources)	17	4	0.6	10.2
27.2 2.3.	Training in radiochemical methods and radioactivity measurements of anthropogenic radionuclides for advanced practitioners	5	5	1	5
28.2 29.2.	Radiation protection for industrial and other practices (radiography) – Refresher Course	2	4	0.4	0.8
28.2.	Radiation protection for industrial and other practices (unsealed sources) – Refresher Course	5	5	0.2	1
28.2.	Radiation protection for industrial and other practices	3	3	0.2	0.6
28.2.	Radiation protection for industrial and other practices (measurement of roadway density and humidity) - Refresher Course	3	4	0.2	0.6
28.2.	Radiation protection for industrial and other practices (sealed sources) – Refresher Course	11	3	0.2	2.2
1.3.	Training Extension for RP Officers	8	2	0.2	1.6
10.4.	Radiation protection for minimum exposed workers at NPP Krško – Refresher Course	5	1	0.2	1
16.4 27.4.	Training in radiochemical methods and radioactivity measurements of anthropogenic radionuclides for advanced practitioners	3	2	2	6
11.5.	Europe Regional Physical Protection and Security Management (Practical Exercise Information)	23	4	0.2	4.6
11.6 22.6.	Training in radiochemical methods and radioactivity measurements of anthropogenic radionuclides for advanced practitioners	5	2	2	10
18.6 22.6.	Fundamentals of nuclear technology	23	4	1	23
3.9 7.9.	Training in radiochemistry and radioactivity measurements for practi- tioners from countries eligible under the JRC Enlargement & Integration policy	5	1	1	5
10.9 10.10.	Basics of nuclear technology, theory	10	11	4.6	46
1.10 3.10.	Radiation protection for industrial and other practices (unsealed sources)	1	5	0.6	0.6
1.10 3.10.	Radiation protection for industrial and other practices (sealed sources)	21	4	0.6	12.6
1.10 12.10.	IAEA Group Fellowship Training Programme on Research Reactors	10	11	2	20
9.10.	Radiation protection for industrial and other practices (unsealed sources) – Refresher Course	3	5	0.4	1.2
9.10.	Radiation protection for industrial and other practices (sealed sources) – Refresher Course	11	4	0.2	2.2

Date	Title of the course	Participants	Lecturers	Weeks	Participants × Weeks
11.10 9.11.	Basics of nuclear technology, systems	16	8	3.4	54.4
11.10.	Training Extension for RP Officers	18	2	0.2	3.6
15.10 26.10.	Training in radiochemical methods and radioactivity measurements of anthropogenic radionuclides for advanced practitioners	6	1	7	42
5.11 (5.4.2013)	Nuclear Technology, Theory	23	19	8	184
19.11 23.11.	Training Course on "Design safety and safety evaluation for NPP SAR - 1W"	13	13	1	13
12.12 13.12.	Use of programs for core analysis (LOADF, SHUFFLE in INCORE-3D)	4	2	0.4	1.6
18.12 19.12.	Radiation protection for Nuclear Medicine Dpt Refresher Course	14	5	0.4	5.6
TOTAL		304	167	54.4	684



Figure 3: Nuclear technology course underway in the Nuclear Training Centre.

INTERNATIONAL PROJECTS

- 1. Registration fees for the OTJE-theory Prof. Igor Jenčič
- 7. FP EURATOM: Permanent fusion exhibition at JSI nuclear training centre 6.1.1-FU; Annex 2 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Prof. Igor Jenčič
- Fusion Expo support action under EFDA work programme, task agreement WP10-PIN-FUSEX

Ministry of Higher Education, Science and Technology Tomaž Skobe, B. Sc.

- 7. FP EURATOM: Public information in the association 6.1.1-FU Ministry of Higher Education, Science and Technology Prof. Igor Jenčič
- Realization of the international workshop: Group fellowship training programme on research reactors (IAEERRI11, IAEERRI11A, IAEERRI12), ICJT, 7.-18. 3. 2011; 7.-18. 11. 2011, 1.-12. 10. 2012
 IAEA - International Atomic Energy Agency

Saša Bobič

 Training and tutoring for experts of the NRAs and their TSOs for developing and strengthening their regulatory and technical capabilities - INSC Project MC.03/10 - LOT 1 ITER-Consult SRL Saša Bobič

R & D GRANTS AND CONTRACTS

1. Trainings of the RZ for foreign market Matejka Južnik, M. Sc.



Figure 4: Society of mathematicians, physicists and astronomers of Slovenia on a traditional visit to the Nuclear Training Centre with its young members that were shown the TRIGA research reactor.



Figure 5: Trainees of the Nuclear Technology course during practical work at the TRIGA research reactor.



 regional training course on the physical protection and security management of radioactive sources, Bled, Slovenia, 9.-11. 5. 2012 Matjaž Koželj, M. Sc.

NEW CONTRACTS

 Implementation of training program "Technology of Nuclear Power Plants - Theory" Gen Energija, d. o. o. Prof. Igor Jenčič

VISITOR FROM ABROAD

1. Dr. Alexander Bychkov, Deputy Director General, IAEA, Vienna, Austria, 6. 11. 2012

STAFF

Researcher

1. Prof. Igor Jenčič, Head Technical officers

- 2. Jure Hribar, B. Sc.
- Jure Hribar, B. Sc.
 Rado Istenič, B. Sc.
- Kado Istellic, B. Sc.
 Matjaž Koželj, M. Sc.
- Matjaz Kozelj, M. Sc.
 Nataša Medved, B. Sc.
- 6. Tomaž Skobe, B. Sc.

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- Matjaž Koželj, Bruno Cvikl, "Comments on the current-voltage interpretation of organic diodes by the model of traps exponentiality distributed in energy", In: *Proceedings*, 48th International Conference on Microelectronics, Devices and Materials & theWorkshop on

 Inplementation of 2012 training program for Krško NPP Krško Nuclear Power Plant Prof. Igor Jenčič

 Implementation of the public information and monitoring of media reports about nuclear energy and GEN Energija, d.o.o. activities Gen Energija, d.o.o. Prof. Igor Jenčič

- 7. Vesna Slapar, B. Sc.
- 8. Luka Tavčar, B. Sc.
- 9. Nina Udir, B. Sc. Technical and administrative staff
- 10 Saša Bobič
- 11. Matejka Južnik, M. Sc.
- 12. Borut Mavec, B. Sc.

Ceramic Microsystems, September 19 - September 21, 2012, Otočec, Slovenia, Darko Belavič, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2012, pp. 163-167.

 Matjaž Koželj, Bruno Cvikl, "On possibilities of neutron detection with organic semicinductor structures", In: *Proceedings*, 21st International Conference Nuclear Energy for New Europe, Ljubljana 2012, September 5-7, Tomaž Žagar, ed., Samo Fürst, ed., Ljubljana, Nuclear Society of Slovenia, 2012, 8 pp.

RADIATION PROTECTION UNIT

SVPIS

The SVPIS has been involved in ionizing-radiation measurements and radiation protection since the commissioning of TRIGA MARK II Research reactor in 1966. The responsibility of SVPIS is the radiation control of all the activities at the Institute dealing with ionizing radiation. Our main task is the supervision of the reactor and the 17 laboratories that use sources of ionising radiation in their research work. More than a hundred different sources are used, such as sealed sources, open sources, X-ray units and the accelerator TANDETRON, which need regulatory control.

The SVPIS is authorized by the Slovenian radiation protection administration to perform control in industrial and research institutions dealing with open or sealed radioactive sources and X-ray units. Furthermore, we are involved in radioactive waste management.

The measurements of dose rate, contamination and gamma spectrometry are performed using an accredited method (EN ISO/IEC 17025).

Personal dosimetry

The personal doses of 130 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters (TLDs). The maximum individual yearly dose was 0.05 mSv. This is only 0.3 % of the regulatory limit for occupational exposure (20 mSv per year) and 5 % of the limit for the general public (1 mSv per year). The collective dose at the JSI in 2012 was 0.41 man mSv.

Supervision of research reactor and laboratories

The controlled area of the Research Reactor, the Hot Cell Facility and the Department of Environmental Sciences were monitored on a weekly basis. During some activities the constant presence of a radiation-protection worker was needed (i.e., for the opening of activated samples or radioactive-waste management). Measurements of dose rate (Figure 1), surface contamination, contamination of different objects and personal contamination were performed routinely. In most cases, no or very low contamination levels could be measured in the controlled areas. Gamma spectrometry was used to monitor solid, liquid, aerosol, and gas samples as well as radioactive waste.

In 2012 we performed 20 inspections in other JSI laboratories. An independent inspection by an external authorized institution was performed in the SVPIS laboratory and two additional laboratories at the JSI. There were no deficiencies recognized that could be important for radiation protection.

At present, 107 sources of radiation are used that require regulatory control. Additionally, 384 low-activity sources are used in various laboratories.

Environmental monitoring of the Reactor Center was performed by

Environmental measurements

Figure 1: Dose-rate measurements at reactor platform

measurements of external radiation levels, measurements of environmental samples and effluent measurements (gas discharges from the reactor operation and liquid discharges into the Sava River).

With environmental TLDs the radiation levels in the surroundings of the reactor and all the premises on the site were monitored. Outside the controlled area only normal, natural background radiation levels could be measured.

Based on the effluent measurements and a conservative, environmental transfer model the effective dose to the reference group in the public was estimated to be less than 1 μ Sv/year. The public exposure in 2012 due to activities at the Reactor Center was insignificant.

Service for outside customers

The Radiation Protection Unit is authorized for supervision measurements and expert assessments in the field of radiation protection. In the past year several radiological control investigations were carried out in industrial and research institutions. Our group has participated in the evaluation of the radiological monitoring of Krško NPP, the research reactor TRIGA and storage for low- and intermediate-level waste in Brinje.

In the scope of international projects we also collaborated in the organization and transport of spent fuel from the Vienna research reactor through Slovenia (Figure 2).





Matjaž Stepišnik, M. Sc.

The fast response of our organisation to repair the failure of a thickness gauge that uses a high-activity caesium source at ACRONI, d.o.o. was also important. Due to excellent cooperation between the JSI, the regulatory authority and the ARAO the device was repaired in a very short time and serious economic damage was prevented.



Figure 2: Left: Radiation-level measurements during the transport of spent nuclear fuel. Right: Radiation measurements during the installation of the thickness gauge at ACRONI d.o.o.

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CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION

CTT

In January 2011 the Center for Technology Transfer and Innovation (CTT) was established at the Jozef Stefan Institute. Its principal activities are the transfer of technology and know-how from the JSI to industry and education, research work in the field of innovation and innovation management, and the implementation of specific technology projects. The TTGroup has been operational since 2010. The TTGroup is a joint technology-transfer office of the Jozef Stefan Institute and the National Institute of Chemistry.

In 2012 the Centre for Technology Transfer and Innovation (CTT) was involved in nine major projects and took on four new EU projects from different funding programme schemes. Within the CIP programme scheme we were involved in the EEN (Enterprise Europe Network) and Slo-Inno-Boost. The project EnvImpact (Increasing the impact of Central-Eastern European environment research results through more effective dissemination and exploitation) was carried out under the EU's 7FP and started a new project TIPS (Enhancing the capacity of EU Transport Projects to transform research results into innovative products and services) under the same programme Head: scheme. Within the Alpine Space Programme we participated with the Alps4EU (Alpine Space Clusters Initiative for Dr. Špela Stres

EU) and began work on the project FIDIAS (Innovative Financial Instruments for Sustainable Development and Alpine Spaces). In the context of South East Europe, we started the project EVLIA (Making full value of good ideas by leveraging Intellectual Assets for financing SMEs in SEE), in the framework of Central Europe. Together with the department CT3 we started to work on the project Central community (Emerging communities for collective innovation and Central Europe). We also carry out the project IPforSMEs (The Role of Intellectual Property (IP) and create regional value through interregional exchange IP) under the Cross-Border Cooperation Slovenia -Italy. We were also involved in national projects: ZS (Scientific meetings, ARRS) and TP PROINCOR (Technology Park Ljubljana). We also carried out some commercial projects of small contract value.

We maintain an online entry point with a set of ISI competencies to communicate with business partners and the general public, http://tehnologije. ijs.si. We were involved in the establishment of a spin-out company and we were supporting researchers in the preparation of two proposals for spin-out companies. In 2012 we dealt with seven invention disclosures and with five patent applications. In 2012 we conducted 21 different cases related to the JSI's intellectual property, we established proper legal basis and contracts in all cases where it was necessary (10 contracts of the new type).

Assistance with intellectual property protection and licensing/commercialization of technologies is performed firstly by the assessment of the technology and market potential; secondly we review the patent databases and thirdly we help researchers protect intellectual property and help them during implementation of the invention in the economy. We carried out a review of the status of all patent applications with the JSI and NIC since 2007, and we evaluated the patents according to the state of the art and potential market. After that assessment there remained 44 technologies: 22 of them are based on patents, 11 of them are from NIC. We run active marketing operations for the 13 best examples of technologies, of which 6 are from JSI and 7 from NIC, in the context of the TT Group.

To assist in the commercialization of the R&D results, the inventors, researchers and entrepreneurs from Slovenia are turning to us. To increase the active collaboration between researchers and industry we organized visits to/from more than 37 companies and the researchers identified over 60 new



Figure 1: The meeting between researchers and business representatives. Photo: M. Trobec

For the implementation in our Center, we acquired four new EU projects in different programme schemes.



Figure 2: JSI Open doors

We visited more than 37 companies. The researchers from the JSI, together with the industrial partners, identified over 60 new development projects.

During the JSI Week of Open Doors there were more than 1300 visitors to the Institute; an additional 47 visits were organized throughout the year, bringing more than 1200 visitors.

In September we organized the 5th International Technology Transfer Conference and gave two awards with a total value of €3000.



Figure 3: Award ceremony on 5th International Technology Transfer Conference

development projects at fourteen companies. We helped several research departments in the submission of European projects.

During the JSI Open Doors event (called the Week of Open Doors since 2010) the Institute was visited by more than 1300 people and they learned a lot about the Institute, and the structure and activities of individual laboratories. In addition, we recorded 47 other visits (and 1200 visitors) from kindergartens, primary schools, high schools, institutions, as well as the individuals from all over Slovenia and abroad. In 2012 a total of 2500 people visited the Institute and learned about the work of the largest research institution in Slovenia.

We also organised field trips for 19 young researchers in two large Slovenian companies, in total 27 young researchers participated in company visits.

Colleagues at the CTT participated, as organizers or co-organizers, at seven events, as well as attending conferences, training sessions and other meetings. A total of 40 task forces and other meetings were carried out, with the aim of establishing an integrated support environment.

We would especially like to highlight the organization of the 5th International Technology Transfer Conference, held from 25 to 27 September, 2012. The conference awarded the prize for the most innovative project. The International Commission of the representatives of venture capital awarded the prize of €3,000 for innovative ideas, coming from the University of Ljubljana and from the National Institute of Chemistry. At the conference we hosted representatives of the Enterprise Europe Network from Croatia, Serbia, Montenegro and Macedonia, and we organized meetings for the companies with them and with researchers from the JSI and NIC.

Organization of conferences, congresses and meetings

- 1. Information sources in Biotechnology, Ljubljana, 2. 2. 2012
- 2. Young researchers 1: Academic Entrepreneurship for young researchers at NIC, Ljubljana, 27. 2. 2012
- 3. Presentation of the last published set of calls in FP 7 and consultation on the successful approach in the preparation of project applications, Ljubljana, 13. 7. 2012
- 4. South-East Enterprise Europe Network Conference, Ljubljana, 25.-26. 9. 2012
- 5. 5th International Technology Transfer Conference, Ljubljana, Maribor, 26.-27. 9. and 3. 10. 2012
- 6. Presentation of call for the Research voucher, Ljubljana, 10. 10. 2012
- 7. Young researchers 2: Academic Entrepreneurship for young researchers at JSI, Ljubljana, 6. 12. 2012

INTERNATIONAL PROJECTS

- Evaluation of industrial projects for italian partner Veneto Innovazione Spa Dr. Špela Stres
- 7. FP⁻ COSMOS: Cooperation of space NCPs as a means to optimise services European Commission Dr. Špela Stres
- 7. FP ENVIMPACT: Increasing the impact of Central-Eastern European environment research results through more effective dissemination and exploitation European Commission Marjeta Trobec, B. Sc.
- 7. FP TIPS: Enhancing the capacity of EU transport projects to transform research results into innovative products and services European Commission
- Dr. Špela Stres
- 5. ACT CLEAN Access to technology and know-how in cleaner production in Central Europe
- European Commission Tanja Zdolšek, B. Sc.
- 6. I3E Promoting innovation in the industrial informatics and embedded systems sectors through networking
 So List Tabaia Constant
- See Joint Tehnical Secretariat Dr. Špela Stres

7. Alps 4 EU

European Commission Dr. Špela Stres

- IPforSMEs Intellectual property for small and medium sized companies Government Office Local Self-Government and Regional Policy Dr. Špela Stres
- FIDIAS innovative financial instruments for sustainable development in Alpine space European Commission Dr. Šnela Stres
- CIP EACI-EIC & IRC Slovenia 2: EIC & IRC services in support of business and innovation
 - European Commission Marieta Trobec, B. Sc.
- II. CIP Slo-Inno-Boost: Slovenian innovation boost; EEN/SPA/09/INO/257213 European Commission
 - Marjeta Trobec, B. Sc.
- Knowledge Transfer: The Road Ahead Prague Empirica - Communication and Technology Research Dr. Spela Stres
- Annual workshop of the European Intellectual Property Teachers' Network (EIPTN), Milan, 12.-13. 7. 2012 Queen Mary, University Of London Dr. Špela Stres

14. CE - Central community-emerging communities for collective innovation in Central Europe European Commission

- Dr. Spela Stres 15. SEE: Making full value of good ideas by leveraging intellectual assets for financing SMEs
 - See Programme Joint Technical Secretariat Dr. Špela Stres

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- Ian Tracey, Coordinator for technology transfer network HEPTech, Science and 2. Technology Facilities Council, London, Great Britain, 21. 11. 2012

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