JSI REPORT P-325 ANNUAL REPORT JUNE 2012



## Annual Report 2011





Annual report 2011

Publisher: Jožef Stefan Institute, Jamova cesta 39, Ljubljana, Slovenia

http://www.ijs.si

Editors: Dr. Luka Šušteršič, Marjan Verč, M. Sc.

Language adviser: Asst. Prof. Paul John McGuiness

ISSN 1318-7392

Photography: Marjan Smerke and departmental archives

Layout: Blaž Corn, B. Sc., Marjan Verč, M. Sc.

Printed by: ABO grafika, d. o. o. , Ljubljana

Ljubljana, June 2012



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## INTRODUCTION

If knowledge is not applied it does not really exist. Not that I think that knowledge is valuable only if it can be consumed, but I believe that the transformation of data and information into knowledge is as demanding as creating music from a series of notes. If we evaluate research with respect to what good it brings, or will bring, to the people, then the dilemma as to whether we should mainly develop basic knowledge or new technologies becomes irrelevant. The impact of scientific research and technological development is the greatest when both basic research and technological development are equal, i.e., balanced, and when they both receive equal social recognition. When this balance is established and the interaction between the two is in place, scientific research and technological development can bring the greatest benefits. Neglecting one at the expense of the other weakens both of them, and this weakening has a negative effect on everything else, not only in the economic, but also in the cultural, social and other fields.

We know that we can achieve this balance by treating basic science and technological development as some kind of connecting vessels; however, we still cannot effectively implement this concept into our lives. This might be so because we seek the solutions, from which only small groups can benefit, or because we do not have enough knowledge and awareness to develop a comprehensive approach to this issue. It is easy, of course, to criticise disinterested and narcissistic scientists or, on the other hand, technologically backward and non-development-oriented companies. But in this way we only minimise and marginalise the excellent results achieved in both scientific research and technological development. I can say, with certainty, that such results have been achieved in environments characteristic for their positive, open-minded and cooperative attitudes, but not in those that lack such qualities.

Unfortunately, it also has to be pointed out that, in the past decade, the organisation and operation of national research institutions were dominated by an attitude that has pushed researchers into the past by at least fifty years, into the situation we had in the 1950s. It is clear that society is being bureaucratised by some obscure players, greatly affecting also scientific research and development. I believe the reason for this process is a deep misunderstanding and ignorance of research and development and of their roles in the modern world. The state has to – as soon as possible and through a dialogue and in cooperation with researchers – introduce more modern and efficient solutions.

To balance the above critical view I also have to point out the positive side of our research and development activities: in recent years the development indicators of the Jožef Stefan Institute have been, in all our areas and despite the economic stagnation in the country, very positive. As a result of winning research and development projects (the Institute obtains all its resources in a competitive way) the number of our employees has increased to record figures; this happened solely due to the employment of young researchers, while the numbers of senior researchers and the staff in the support services have been on a slight decrease. An important outcome of such a development was a significant increase in the transfer of young PhD researchers to industry, which was really a historical shift. In addition, by the end of last year the economic crisis had no fatal influence on our projects carried out for industry or for other direct users.

However, looking at it from today's perspective, the economic crisis has not abated, but it is continuing with an even greater impact, so that the forecast for 2012 and 2013 is not at all optimistic. Our biggest worry is that young, ambitious and talented people will be without opportunities and such a situation will lead to irreparable consequences. In my view there is no other issue as important as this one.

Prof. Jadran Lenarčič Director of the Jožef Stefan Institute



Adressing the Institute employees at the end of the year



## 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, XeF<sub>6</sub>, 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

 $\sim$  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) Prof. Stanislav Strmčnik, 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. Se Mass Spectrometry Centre Dr. Dušan Žigon National Centre for Microstructure and Surface Analysis Prof. Miran Čeh National High Resolution NMR Spectroscopy Prof. Janez Dolinšek **Centre for Protein Structure** Prof. Dušan Turk Nanolitography and nanoscopy Prof. Dragan Mihailović Center 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) Jože Kašman, B. Sc., Darko Korbar, M. Sc., MBA Finance and Accounting (U-4) Regina Gruden, B. Econ. Public Relations Polona Strnad, B. Sc. Technical Services (TS) Slavko Zalar, B. Sc., Boštjan 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 Competence Centre (SEITCE)					
Jožef Stefan International Postgraduate School	Development Centre for Hydrogen 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	Center 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

Darko Korbar, M. Sc., MBA (*to 31 October 2011*) Jože Kašman, B. Sc. (*from 1 November 2011*) Daša Modic Gorjup, LL. B. Dr. Boris Pukl Marta Slokan, LL. B.

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since 27 January 2011 Prof. Dragan Dragoljub Mihailovič, President Prof. Denis Arčon Prof. Milena Horvat Prof. Spomenka Kobe Prof. Borka Džonova Jerman Blažič Prof. Jadran Lenarčič Prof. Andrej Likar Prof. Borut Mavko Prof. Marko Mikuž Prof. Ingrid Milošev, Deputy President Asst. Prof. Mihael Mohorčič, Deputy President Prof. Peter Prelovšek Prof. Danilo Suvorov Prof. Vito Turk Asst. Prof. Leon Žlajpah

# STAFF QUALIFICATIONS

## 1949-2011



## RECIPIENTS OF THE JSI AWARDS AND TITLES

## HONORARY MEMBERS

Prof. Robert Blinc<sup>+</sup>, 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

Prof. Milan Osredkar<sup>+</sup>, Director of the Jožef Stefan Institute from 1963 to 1975 (1919 - 2003)
 Prof. Anton Peterlin<sup>+</sup>, 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
Prof. Neil Bartlett<sup>\*</sup>, University of California, Berkeley, California, USA
Prof. John H. Beynon, University of Wales Swansea, Swansea, United Kingdom
Prof. Wolfram Bode, Max-Planck-Institut für Biochemie, Munich, Germany
Prof. Oscar D. Bonner<sup>\*</sup>, University of South Carolina, Columbia, South Carolina, USA
Dr. Horst Borrmann, Max-Planck-Institut für chemische Physik fester Stoffe,

Dresden, Germany

Prof. Henrik Buchowsky, Politechnika Warszawska, Warszawa, Poland Prof. Rüdiger Dillmann, Karlsruher Institut für Technologie, Karlsruhe, Germany Prof. Joseph W. Doane, Liquid Crystal Institute, Kent State University, Kent, Ohio, USA Prof. Hans Fritz, Universität München, Munich, Germany Prof. Oskar Glemser<sup>‡</sup>, Universität Göttingen, Göttingen, Germany Prof. Paul Hagenmuller, Université de Bordeaux I, Bordeaux, France Prof. John Holloway, University of Leicester, Leicester, United Kingdom Prof. Rudolf Hoppe, Universität Giessen, Giessen, Germany Prof. Robert J. Jaeger<sup>‡</sup>, National Institute on Disability and Rehabilitation Research, US Department of Education, Washington, D. C., USA Prof. Nikola Kallay, University of Zagreb, Zagreb, Croatia Prof. Nobuhiko Katunuma, Tokushima Bunri University, Tokushima, Japan Prof. Raymond Kind, ETH, Zurich, Switzerland Prof. Jože Koller, National Institute of Chemistry, Ljubljana, Slovenia Prof. Rüdiger Mews, Universität Bremen, Bremen, Germany Prof. Donald Michie<sup>+</sup>, Edinburgh University, Edinburgh, United Kingdom Dr. Fani Milia, National Centre for Scientific Research "Demokritos", Athens, Greece

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Prof. Vlado Valković, Zagreb, Croatia Prof. John Waugh, M.I.T., Cambridge, Massachusetts, USA

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Prof. Andrej Župančič<sup>⊕</sup>, Slovenian Academy of Sciences and Arts, Ljubljana, Slovenia

# INTERNATIONAL ADVISORY BOARD

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

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- Prof. H. Eugene Stanley, Boston University, Boston, Massachusetts, USA
- Prof. Thomas Walcher, Universität Mainz, Mainz, Germany

## DELEGATIONS AND VISITORS

- Prof. Thomas A. Henzinger, President of the Institute of Science and Technology Austria (IST Austria), Klosterneuburg, Austria, 6 April 2011
- H. E. Mr Toshimitsu Ishigure, Ambassador of Japan, Embassy of Japan, Ljubljana, Slovenia, 8 April 2011,
- Prof. John Hollerbach, University of Utah, Salt Lake City, Utah, USA, 27 June 2011
- Prof. Harry Kroto, Nobel Prize Winner 1996, Florida State University, Tallahassee, Florida, USA, 20 July 2011
- Dr. Danilo Türk, President of the Republic of Slovenia, 17 October 2011
- Prof. Erkki KM Leppävuori, President & CEO, VTT Technical Research Centre of Finland, Finland, 23 November 2011
- H. E. Mr Toshimitsu Ishigure, the Ambassador of Japan, Embassy of Japan, Ljubljana, Slovenia, 20 December 2011



Dr. Danilo Türk, President of the Republic of Slovenia

# 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 KNOWLEDGE, RESEARCH POTENTIAL, SCIENCE AND SOCIETY, INCO (HORIZONTAL), DEVELOPMENT OF POLICIES)	75
7. FP - EURATOM	24
6. FP (LIFESCIHEALTH, IST, NMP, AERO, TREN, SPACE, FOOD, ENERGY, TRANSPORT, GLOBAL, CITIZENS, SSP, NEST, SME, INCO, ERA-NET, MOBILITY, INFRASTRUCTURES, SCIENCE AND SOCIETY, RESEARCH/INNOVATION POLICIES)	5
IEE	7
CIP	3
LEONARDO DA VINCI	2
E-CONTENTPLUS, PHEA	3
EMRP	4
ESA (PECS)	4
EUREKA	3
COST	25
NATO (SfP, CLG)	1
IAEA	10
LIFE PLUS	1
ERA-NET (MATERA, MNT, MNT II, SEE, ERASME)	9
SEE, SEE.ERA.NET PLUS, CEE, ALPINE SPACE OPERATIONAL PR.	5
OTHERS (DELPHI, ATLAS, CERN RD-39, CERN RD-42, CERN RD-50, BELLE, BELLE II, CIMA, SCOPES, IEEE-RAS, EUROSTARS, MŠŠ, SIM-RIS, WAEGNER, NET WORDS, EUSAS, ARTEMIS, SERENA - OECD/NEA, CAMP, F4E, EURADOS, SLOVENIA - RTD AUDIT, ERASMUS, MED, HFSPO)	26
TOTAL	207

<b>Bilateral cooperation</b>	No. of projects	<b>Bilateral cooperation</b>	No. of projects
Albania	1	Hungary	7
Argentine	2	Mexico	1
Austria	9	Germany	2
Belgium	13	The Netherlands	2
Bulgaria	2	Norway	2
Bosnia and Herzegovina	2	Poland	5
Brazil	3	Portugal	2
Czech Republic	2	Romania	2
Montenegro	3	Russia	1
Finland	2	Slovakia	1
France (PROTEUS - 6)	7	Serbia	6
Croatia	10	Sweden	1
Italy	2	Turkey	2
Japan	8	Ukraine	1
China	15	Great Britain	2
Korea	3	USA	17
		ΤΟΤΑΙ	128

## INTERNATIONAL COOPERATION AGREEMENTS

In 2011, cooperation agreements were signed between the Jožef Stefan Institute and:

- 1. Merck KGaA, Darmstadt, Germany
- 2. Oslo University, Department of Physics, Norway; Lund University, Department of Physics, Sweden; Copenhagen University, Niels-Bohr Institute, Denmark; University of Helsinki, Helsinki Institute of Physics, Finland; Uppsala University, Department of Physics and Astronomy, Sweden; NIIF, Nemzeti Információs Infrastruktúra Fejlesztési Intézet, Hungary; Swiss National Grid association (SwiNG), Switzerland; Pavol Jozef Šafárik University in Košice, UPJS, Slovakia; Ukrainian National Grid, Ukraine; Lithuanian National Grid (LitGrid), Lithuania
- The National Physical Laboratory (NPL), NPL Management Ltd, Teddington, Middx, United Kingdom
- 4. Enviros Consulting Limited, Wolverhampton, Quintessa Limited, Oxon, Great Britain

- 5. Hungarian Academy of Sciences, Institute for Geochemical Research, Budapest, Hungary
- 6. Faculty of Geography, M.V. Lomonosov Moscow State University, Moscow, Russian Federation
- 7. FIR e.V an der RWTH Aachen, Aachen, Germany
- 8. University of York, York, Great Britain
- 9. Halbleiter Deutschland GmbH, Munich, Germany
- 10. Akademija nauka i umjetnosti Bosne i Hercegovine, Centar za koordinaciju medicinskih istraživanja, Sarajevo, Bosnia in Herzegovina
- 11. Quant Technologies, LLC, Blaine, MN, USA
- 12. Morphoplant GmbH, Bochum, Germany

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### MENTORING

#### Doctoral theses

- Petra Avanzo Caglič, Biochemical and biological properties of cnispin, a new serine protease inhibitor from muschroom Clitocybe nebularis (mentor Borut Štrukelj; co-mentor dr. Jerica Sabotič).
- 2. Meleq Bahtijari, *Radon in Kosovo* (mentor Peter Stegnar; co-mentor Zahadin Shemsidini).
- Miloš Beković, Development of measurement procedures for determining the magnetic losses of magnetic fluids (mentor Anton Hamler; co-mentor Mihael Drofenik).
- 4. Rok Bojanc, *Models for providing security in business information systems* (mentor Borka Jerman Blažič).
- Pavle Boškoski, Condition monitoring of mechanical drives: feature extraction and fault diagnosis methods (mentor Đani Juričić; co-mentor Mile Stankovski).
- Tadej Debevec, The use of normobaric hypoxia and hyperoxia for the enhancement of sea level and/or altitude exercise performance (mentor Igor B. Mekjavić; co-mentors Blaž Jereb, Stylianos N. Kounalakis).
- 7. Miha Devetak, *Self-assembly of guanosine derivates on surfaces* (mentor Irena Drevenšek Olenik).
- 8. Ivica Dimitrovski, *Generic system for content based image retrieval* (mentor Suzana Loškovska; co-mentor Sašo Džeroski).
- Urban Došler, The synthesis and characterization of glass-ceramic based on ternary system MgO-B<sub>2</sub>O<sub>3</sub>SiO<sub>2</sub> (mentor Danilo Suvorov; co-mentor Marjeta Maček Kržmanc).
- Blaž Fortuna, Semi-automatic ontology construction (mentor Dunja Mladenić).
- 11. Matej Gašperin, Parameter estimation of nonlinear dynamic systems with application to failure prognostics (mentor Đani Juričić).
- Gorazd Golob, Elastomer surface energy modification applying oxygen and nitrogen plasma treatment with laser deactivation of the surface (mentors Mladen Lovreček, Miran Mozetič).
- Martin Gorjan, Mid-infrared erbium doped fiber laser (mentor Martin Čopič; co-mentor Marko Marinček).
- Biljana Govedarica, Evaluation of mechanical and surface properties of pharmaceutical materials and products on a single particle level by atomic force microscopy (mentor Stane Srčič; co-mentor Miha Škarabot).
- 15. Andrej Hrovat, *Radio wave propagation in special environments* (mentor Gorazd Kandus; co-mentor Tomaž Javornik).
- David Jezeršek, Ion beam analysis of geometrically structured samples (mentor Žiga Šmit).
- Michail Keramidas, Normobaric Hyperoxia: Haemodynamic responses to acute and long-term exposure (mentor Igor B. Mekjavić; co-mentors Ola Eiken, Nickos D. Geladas).
- Andrej Kobler, New methods of processing aerial laser scanner data for forest ecosystem monitoring (mentor Krištof Oštir; co-mentor Sašo Džeroski).
- Dragi Kocev, Ensembles for predicting structured outputs (mentor Sašo Džeroski).
- 20. Katja König, *The production of advanced ceramic materials by electrophoretic deposition* (mentor Spomenka Kobe; co-mentors Saša Novak Krmpotič, Aldo R. Boccaccini).
- 21. Alenka Kužnik, *The mechanism activation and inhibition of endosomal Tolllike receptors* (mentor Roman Jerala; co-mentor Janko Kos).
- Tanja Ljubič Mlakar, Mercury in the process of cement clinker production and emission control (mentor Milena Horvat).

- 23. Mathieu Lu-Dac, *Phase slip phenomena and vortex dynamics in mesoscopic superconductors* (mentor Viktor V. Kabanov).
- 24. Satja Lumbar, *Predictive control of aircrafts based on visual servoing* (mentor Drago Matko; co-mentor Stanko Strmčnik).
- 25. Boštjan Maček, Measurement of luminosity in ATLAS spectrometer with beam conditions monitor (mentor Marko Mikuž; co-mentor Andrej Gorišek).
- 26. Aljoša Maglica, *Innovative electroconductive ceramic composites based on Si<sub>z</sub>N<sub>a</sub>* (mentor Tomaž Kosmač; co-mentor Kristoffer Krnel).
- 27. Martin Mihajlov, *Usable authentication with recognition-based graphical passwords* (mentor Borka Jerman Blažič; co-mentor Tomaž Klobučar).
- 28. Bojana Mirković, *Regulation of exopeptidase and endopeptidase activity of cathepsin B* (mentor Janko Kos).
- Petra Nikolić, Gene expression patterns in grapevine leafs infected with phytoplasma associated with bois noir disease (mentor Marina Dermastia; co-mentor Kristina Gruden).
- Inna Novalija, Ontology extension using text mining for news analysis (mentor Dunja Mladenić).
- Roman Pačnik, Hydraulic load cells for measurement of small loads (mentor Franc Novak; co-mentor Marija Kosec).
- 32. Stane Pajk, *Influence of some cholesterol oxidation products on the structure of model membranes* (mentor Slavko Pečar; co-mentor Janez Štrancar).
- Viljem Pavlovič, Modelling of alpha-acid content early prediction by hops (Humulus lupulus L.) with machine learning models (mentor Črtomir Rozman; co-mentor Marko Bohanec).
- 34. **Igor Perkon**, *Analysis of whisker dynamics by tracking of non rigid open curves* (mentor Jurij F. Tasič; co-mentor Mathew Diamond).
- Larisa Pograjc, Impact of nutrition and physical stress on selenium status at soldiers (mentor Vekoslava Stibilj; co-mentor Ingrid Falnoga).
- 36. Aleksander Pur, *Model for monitoring and assessment of a public health care network* (mentor Marko Bohanec).
- Mojca Rangus, The study of structural characteristics and formation of microporous and mesoporous materials (mentor Gregor Mali; co-mentor Janez Seliger).
- Matjaž Ravnikar, Research of recombinant probiotics and interactions between probiotic lactic acid bacteria and drugs (mentor Borut Štrukelj; co-mentor Mojca Lunder).
- Ana Rotter, Development and implementation of system biology tools: a case study of plant physiology data analysis (mentor Andrej Blejec; co-mentor Kristina Gruden).
- 40. Mehdi M. Saghafi, Donepezil and galantamin as a preventive protection against intoxocation with diizopropilfluorofosfat inhibitor of the enzyme AChE (mentor Fajko Bajrović; co-mentor Borut Štrukelj).
- Urban Simončič, Modeling of radiopharmaceuticals uptake into the tumor: optimization of the method and its application in the clinical studies (mentor Robert Jeraj).
- 42. Jure Strle, *Self-assembled MoSI nanowire networks and their properties* (mentor Dragan Mihailović).
- Katarina Susman, Pojem faznega prehoda pri pouku fizike (mentor Mojca Čepič).
- Katja Škerget, Contribution to understanding of the mechanism of amyloid fibril formation and its effects on the cell (mentor Eva Žerovnik; co-mentor Uroš Petrovič).
- 45. **Denis Špelič**, *Lossless compression of segmented voxel data* (mentor Borut Žalik; co-mentor Franc Novak).
- 46. Marko Štrok, *Migration of critical radionuclides in the area of former uranium mine Žirovski vrh* (mentor Borut Smodiš).

- Martina Šturm, Nitrate migration in plant-soil-groundwater sistem (mentor Sonja Lojen).
- 48. Tea Toplišek, *Ceramic composites with long silicon-carbide fibers* (mentor Spomenka Kobe).
- Mitja Uršič, Modelling of solidification effects in fuel coolant interactions (mentor Borut Mavko; co-mentor Matjaž Leskovar).
- Mitja Vahčič, Development of analytical methods for speciation of organotin compounds in environmental samples using gas chromatography and mass spectrometry (mentor Janez Ščančar).
- Tjaša Vrlinič, Development of new anti-bioadhesive surfaces for specific neurodegenerative agents (mentor Miran Mozetič; co-mentor Fabienne Poncin-Epaillard).
- 52. Urška Zapušek Novak, *Preparation of artificial soil mixtures with sewage sludges* (mentor Domen Leštan; co-mentor Radmila Milačič).
- 53. Kristina Žagar, Synthesis and characterization of perovskite nanostructures (mentor Miran Čeh).

#### Master's theses

- 1. **Robert Čebron**, *Design of an information system to support education in the secondary school* (mentor Bojan Cestnik).
- Vitko Črep, Information system for the management of multi-residential buildings and market opportunities for housing managers (mentor Bojan Cestnik).
- 3. Hristijan Gjoreski, *Adaptive human activity recognition and fall detection using wearable sensors* (mentor Matjaž Gams).
- Andrej Jerman Blažič, Educational web applications in vocational education and training in Slovenia (mentor Franc Novak).
- 5. Silvester Jeršič, *The use of UML in procedures of standards ISO 9001 and 14001* (mentor Bojan Cestnik).
- 6. Tadej Kodelja, *Simulation of system dynamics models with Simulink software* (mentor Juš Kocijan).
- Nejc Mekiš, Sacroiliac joint imaging : achieving dose reduction with PA projection (mentor Peter Stegnar; co-mentor Igor Kocijančič).
- Marijan Merljak, Implementing CRM into Business Operations (mentor Bojan Cestnik).
- Cândida Radicchi de Oliveira Alméri, Environmental impacts of aluminium and chromium in bauxide ore and red mud (mentor Janez Ščančar; comentor Radmila Milačič).
- Sweety Karta Ram, Sustainable agriculture in India : need and prospects with particular reference to the state of Punjab (mentors Ivo Šlaus, Peter Stanovnik, Matej Stopar, Gojmir Lahajnar).
- Edvin Raubar, Increasing productivity of ship-to-shore cranes in Port of Koper using advanced electronic systems (mentor Damir Vrančić; co-mentor Đani Juričić).
- Janko Skok, Impacts of forest management on biodiversity : small mammals in the fir-beech forest of Mt. Snežnik as a model group (mentor Boris Kryštufek; co-mentor Marko Debeljak).
- Vidojka Srebrnič, Optimization of vegetable food supply using linear programming (mentor Bogdan Filipič).
- 14. Milen Tewolde, *Functional characterisation of TDP-43 in relevance to ALS* (mentor Boris Rogelj; co-mentor Jacqueline Mitchell).
- Neža Turnšek, Molecular basis of colorado potato beetle (Leptinotarsa decemlineata) response to plant defense response (mentor Kristina Gruden).
- 16. Li Xiaobin, *Implementing DEXi evaluation models in Decision Deck platform* (mentor Marko Bohanec).
- Iztok Zajc, Renewal of an information system for logistic support of firefighting interventions (mentor Bojan Cestnik).

Bologna master's theses

- Petra Barber, Use of multi-attribute decision support model in public procurement (mentor Marko Bohanec; co-mentor Ljupčo Todorovski).
- 2. Luka Cmok, Dynamic light scattering in suspensions of ferroelectric nanoparticles in liquid crystals close to nematic to smetic A phase transition (mentor Alenka Mertelj).
- 3. Raphaël Connes, *Scaling of simualtion of hydrogen combustion with ASTEC computer code from containment experimental facility to actual containment* (mentor Ivo Kljenak).
- 4. Adrien Giacosa, *Steam explosions analysis in reactor conditions* (mentor Matjaž Leskovar).
- Jurij Gorjanc, The effectivity of cold induced vasodilatation as predicting factor for freezing cold injury (mentor Metka Milčinski; co-mentor Igor B. Mekjavić).
- Staša Györköš, An introduction of the new approach to the designing of continuous model for the purpose of stochastic inventory control (mentor Damir Vrančić; co-mentor Dejan Dragan).

- Marko Intihar, Path planing in the process of acquistion of biological samples in the General hospital Celje (mentor Đani Juričić; co-mentor Dejan Dragan).
- 8. Grega Medved, The development of sophisticated inventory management policies with variable demand accompanied with a comparative analysis of obtained results (mentor Damir Vrančić; co-mentor Dejan Dragan).
- Alexandra Moraru, Enrichment of sensor descriptions and measurements using semantic technologies (mentor Dunja Mladenić).
- 10. Maria Porcius, *Topology design and accessibility provision in large scale wireless mesh networks* (mentor Mihael Mohorčič).
- 11. Helena Razpotnik, *Researches of porcelain scrap application in alumina porcelain C-120* (mentor Marija Kosec; co-mentors Janez Holc, Ivan Lavrač).
- 12. Tea Vizinger, *Development of the heuristic algorithm in the process of the biological material acquisition scheduling* (mentor Đani Juričić; co-mentor Dejan Dragan).
- Milena Zorko, Self-assembled structures based on monodisperse spherical silica particles (mentor Saša Novak Krmpotič; co-mentor Miran Gaberšček).

# ART EXHIBITIONS AT THE JSI

Hommage à Zoran Kržišnik, 26 January-17 February Mojca Zlokarnik, 21 February-17 March Dragica Čadež, 21 March-14 April Milan Erič, 18 April-12 May Jurij Kalan, 16 May-9 June Darko Slavec, 13 June-7 July Ljubljana Fine Artist Society, 11 July-1 September Nuša in Boštjan Lapajne, 5 September-29 September Aleksej Kobal, 3 October-27 October Maja Lubi, 2 November-24 November Ludvik Pandur, 28 November-15 December Marko Lakovič, 19 December-13 January 2012



Prof. Jadran Lenarčič, Director of the JSI, and Prof. Dragica Čadež at the opening of the exhibition of her works

# INSTITUTE COLLOQUIA

20 January 2011: Schahram Dustdar Information Systems Institute, Vienna University of Technology Socially enhanced Services Computing

2 March 2011: **Rajmund Krivec** Jožef Stefan Institute *Physics in six dimensions: from fusion research to aircraft accident simulations* 

21 March 2011: **Janez Dolinšek** Faculty of Mathematics and Physics, University of Ljubljana and Jožef Stefan Institute *Complex metallic alloys: from quasicrystals to smart materials* 

22 March 2011: **Rüdiger Dillman** Karlsruhe Institute of Technology *From elementary sensorimotor operations to complex manipulation tasks in humanoid robots* 

23 March 2011: **Miha Drofenik** Jožef Stefan Institute *Synthesis and application of magnetic nanoparticles* 

6 April 2011: **Tom Henzinger** IST Austria *Games, Time, and Probabilities: Models and Algorithms for System Design and Analysis* 

20 April 2011: **Bogdan Pucelj** Jožef Stefan Institute **Černobil (1986) – Fukushima (2011)** 

18 May 2011: **Ingrid Milošev** Jožef Stefan Institute, Orthopaedic Hospital Valdoltra **Studies on biocompatible materials and orthopedic implants** 

25 May 2011: **Leon Cizelj** Jožef Stefan Institute *Nuclear power plant in Fukushima after the earthquake and tsunami on 11 March 2011* 

8 June 2011: **Franci Demšar** ARRS - Slovenian Research Agency *Transparency in public sector: examples in science, international relations and defense*  27 June 2011: **John M. Hollerbach** University of Utah, ZDA *Locomotion Interface for Outdoor Virtual Environments* 

29 June 2011: **Iztok Tiselj** Jožef Stefan Institute *Condensation induced water hammer* 

7 September 2011: **Mamoru Senna** Keio University, Japan *New aspects of processing nanomaterials under mechanical stressing* 

21 September 2011: **Wolfgang Porod** Dept. of Electrical Engineering, University of Notre Dame, U.S.A *NanoMagnet Logic* 

28 September 2011: **Marjan Kromar** Jožef Stefan Institute *Application of the reactivity coefficient method for the nuclear design calculations of PWRs* 

12 October 2011: **Gil Rosenman** School of Electrical Engineering - Department of Physical Electronics, Tel Aviv University, Israel *Biological and Bioinspired Peptide Nanostructures: Basic Physics and Applications* 

26 October 2011: **Iztok Čadež** Jožef Stefan Institute *Collisions of atomic particles* 

2 November 2011: **Sean Fain** University of Wisconsin – Madison, Madison, USA *Methodology and applications of magnetic resonance imaging (MRI)* with hyperpolarized C-13 and He-3 contrast agents

16 November 2011: **Nives Ogrinc** Jožef Stefan Institute **Stable isotopes in theory and practice** 

14 December 2011: **Božidar Šarler** University of Nova Gorica *About Stefan's studies of multiphase systems* 

# FINANCING

## REVENUES JSI (€) AND NUMBER OF PROJECTS

		Contribution		Contribution		No. of Projects
	2011	2011	2010	2010	Index 2011/2010	in 2011
National Agencies and Ministries	37,946,161	75.6 %	34,433,391	73.9 %	110.2	528
National Market	4,682,766	9.3 %	5,748,309	12.3 %	81.5	219
International Market	6,968,502	13.9 %	5,820,943	12.5 %	119.7	330
Other Revenues	601,959	1.2 %	622,278	1.3 %	96.7	
TOTAL	50,199,388	100.0 %	46,624,921	100.00 %	107.7	1077



## POSTGRADUATES FINANCED

1985-2011





## JSI UNDERGRADUATE SCHOLARSHIPS

1977-2011

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
TOTAL	381	90	409	17	6	7	2	60	452	27	20	11	11	1493

FMF FKKT (Uni-Lj)	Faculty of Mathematics and Physics, University of Ljubljana Faculty of Chemistry and Chemical Technology, University of Ljubljana	FRI FG	Faculty of Computer and Information Science, University of Ljubljana Faculty of Civil Engineering, University of Maribor
FKKT (Uni-Mb)	Faculty of Chemistry and Chemical Technology, University of Maribor	FERI	Faculty of Electrical Engineering and Computer Science. University
NTF	Faculty of Natural Sciences and Engineering, University of Ljubljana		of Maribor
FDV	Faculty of Social Sciences, University of Ljubljana	UNG	University of Nova Gorica
FA	Faculty of Administration, University of Ljubljana	IPS	Jožef Stefan International Postgraduate School
BF	Biotechnical Faculty, University of Ljubljana	Other UNI LJ	Faculty of Pharmacy, Faculty of Mechanical Engineering, Faculty of
FE	Faculty of Electrical Engineering, University of Ljubljana		Economics, Faculty of Medicine, University of Ljubljana

## **COMPLETED THESES**

## UNTIL 2011

Year	Ph. D. Theses	M. Sc. Theses	Total	Year	Ph. D. Theses	M. Sc. Theses	Total
1962	15	6	21	1987	18	21	39
1963	7		7	1988	12	26	38
1964	7	2	9	1989	15	33	48
1965	16		16	1990	16	41	57
1966	2		2	1991	22	47	69
1967		8	8	1992	19	42	61
1968	4	8	12	1993	28	36	64
1969	3	6	9	1994	27	37	64
1970	2	12	14	1995	34	22	56
1971	7	6	13	1996	38	25	63
1972	11	24	35	1997	29	23	52
1973	8	14	22	1998	21	20	41
1974	21	10	31	1999	33	29	62
1975	10	20	30	2000	36	27	63
1976	6	31	37	2001	31	28	59
1977	5	16	21	2002	29	19	48
1978	10	20	30	2003	41	19	60
1979	7	11	18	2004	31	20	51
1980	13	10	23	2005	22	7	29
1981	12	15	27	2006	22	2	24
1982	13	18	31	2007	26	7	33
1983	5	10	15	2008	29	5	34
1984	14	17	31	2009	30	7	37
1985	6	14	20	2010	33	5	38
1986	8	15	23	2011	31	2	33
				TOTAL	885	843	1728



# PATENTS GRANTED

- Laser system for medical removal of body tissue Matjaž Lukač, Marko Marinček, Marko Kazič, Karolj Nemes Patent No. US7867224 (B2), United States Patent and Trademark Office, 11.1.2011.
- Process for the synthesis of nanotubes and fullerene-like nanostructures of transition metal dichalcogenides, quasi one-dimensional structures of transition metals and oxides of transition metals Aleš Mrzel, Maja Remškar, Adolf Jesih, Marko Viršek Patent No. US8007756 (B2), United States Patent and Trademark Office,

30.8.2011.

- Method for operating a laser system for bleaching teeth Matjaž Lukač, Boris Cenčič Patent No. US8011923 (B2), United States Patent and Trademark Office, 6.9.2011.
- Metamaterials and resonant materials based on liquid crystal dispersions of colloidal particles and nanoparticles Igor Muševič, Miha Škarabot, Slobodan Žumer, Miha Ravnik Patent No. EP1975656 (B1), European Patent Office, 8.6.2011.
- Multistable liquid crystal device Theo Rasing, Sergiy Lazarenko, Igor Muševič, Miha Škarabot, Marko Uplaznik Patent No. EP1927885 (B1), European Patent Office, 27.7.2011.
- Laser system for medical and cosmetic applications Karolj Nemes, Matjaž Lukač Patent No. EP2030586 (B1), European Patent Office, 11.5.2011.
- Procedure for synthesis of threadlike tungsten oxide W5014 Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih Patent No. EP2114827 (B1), European Patent Office, 16.2.2011.
- Process for applying adhesion coatings to a substrate Tomaž Kosmač, Kristoffer Krnel, Andraž Kocjan, Peter Jevnikar Patent No. EP2170244 (B1), European Patent Office, 30.3.2011.

- 9. Method for synthesis of magnetic liposomes in electric field Kristina Eleršič, Miran Mozetič, Alenka Vesel, Janez Pavlič, Aleš Iglič, Andrej Žnidaršič, Aljoša Košak
  - Patent No. SI23095 (A), Slovenian Intellectual Property Office, 31.1.2011.
- Photocatalytic TiO<sub>2</sub> coatings on superparamagnetic carriers and procedure of their production Darko Makovec, Dejan Verhovšek, Marjan Sajko

Patent No. SI23210 (A), Slovenian Intellectual Property Office, 31.5.2011.

 Rutile nanoparticles and procedure for synthesis of rutile nanoparticles Dejan Verhovšek, Tatjana Rožman, Miran Čeh, Pavel Blagotinšek, Sašo Šturm, Kristina Žagar

Patent No. SI23218 (A), Slovenian Intellectual Property Office, 31.5.2011.

12. Anatase nanoparticles and procedure for synthesis of anatase nanoparticles Dejan Verhovšek, Tomi Gominšek, Miran Čeh, Pavel Blagotinšek, Sašo Šturm, Kristina Žagar

Patent No. SI23219 (A), Slovenian Intellectual Property Office, 31.5.2011.

 Bioactive and photocatalytic coating on metal implants and a process of preparing thereof
 Cata Numb. Natata Dan antal

Saša Novak, Nataša Drnovšek

Patent No. SI23312 (A), Slovenian Intellectual Property Office, 19.3.2011.

14. The use of glycosidases and glycosiltransferases for increased production of proteins

David Dobnik, Špela Baebler, Jana Žel, Kristina Gruden, Dejan Štebih Patent No. SI23374 (A), Slovenian Intellectual Property Office, 30.11.2011.

 Improved magnetocaloric material and procedure of its manufacture Benjamin Podmiljšak, Paul John McGuiness, Spomenka Kobe Patent No. SI23405 (A), Slovenian Intellectual Property Office, 30.12.2011.

# AWARDS AND APPOINTMENTS

## AWARDS MADE TO JSI RESEARCHERS BY THE REPUBLIC OF SLOVENIA

#### Zois Award and Zois Certificate of Recognition

#### Gabrijel Kernel

Presented with the Zois Award for lifetime achievement in physics.

#### Boris Žemva

Presented with the Zois Award for lifetime work on the field of inorganic fluorine chemistry.

#### Boris Turk

Presented with the Zois Award for highest scientific research contributions in the field of transmission of signals with proteases.

#### Ingrid Milošev

Presented with the Zois Certificate of Recognition for significant achievements in research of biocompatible materials and experimental orthopaedics in 2011.

#### Puh Certificate of Recognition

#### Uroš Cvelbar (JSI), Miran Mozetič (JSI), Ludvik Kumar (Kolektor, Idrija)

Presented with the Puh Certificate of Recognition for innovations, development achievements and application of scientific discoveries in industrial practice.

### JSI AWARDS AND APPOINTMENTS

#### The Jožef Stefan Golden Emblem Prize

presented to the following for doctoral theses with high impact :

#### Mitja Nemec

Predictive methods in controlled three-phase power converters

#### Petra Kocbek

Development of nanosystems for enhancing dissolution rate of poorly soluble drugs and active targeting of tumor cells

Miha Ravnik Colloidal structures confined to thin nematic layers

## SELECTED OTHER AWARDS TO JSI RESEARCHERS

Alojzij Franc Kodre, Gold Medal of the University of Ljubljana for scientific, educational and organizational work at the Faculty of Physics

Matjaž Vencelj, Fruitful collaboration and business partnership award, Ljubljana, Fotona d.d.

Marta Lavrič, Ferbar Prize, Ljubljana, Faculty of Education, Liquid crystal elastomers.



The recipients of Zois awards and recognitions

Igor Muševič, Mentor of the year 2011, Ljubljana, Slovenian Society of Young Researchers

Marija Kosec, MIDEM acknowledgement, ceremony at the 25th Academy of the Society for Microelectronics, Electronic Components and Materials, Ljubljana, Slovenia, May 26, 2011

Marin Berovič, Darko Makovec, 2nd award for innovation at 4th International Conference of Technology Transfer, Ljubljana, IJS, Magnetisation of wine yeast and separation in production of sparkling wine.

**Slavko Kralj**, 3. award for innovation UL; Dean's award for best innovation at UL, Ljubljana, proposer Ljubljana University Incubator (LUI) and University of Ljubljana (UL), Multifunctional nanoparticles for biomedical applications.

Andreja Šestan, Award for contribution to the sustainable development of society for the year 2010, Ljubljana, The Slovene Human Resources and Scholarship Fund, Microstructure characteristics of materials based on Ni-GDC and GDC prepared by citrate-nitrate combustion synthesis.

Vojka Žunič, Award for contribution to the sustainable development of society for the year 2010, Ljubljana, The Slovene Human Resources and Scholarship Fund, Sol-gel synthesis of TiO2 nano-powders which are photocatalytically active under visible light irradiation.

**Radmila Milačič**, The Pregl Award for Exceptional Achievements for important scientific contributions in the field of speciation of elements, Ljubljana, Slovenia, 20 June 2011.

Jerica Sabotič, Sara Žigon, Faculty Prešeren Award to the students of Faculty of Pharmacy, of the University of Ljubljana in 2011, Ljubljana.

Andrej Debenjak, received Prof. Vratislav Bedjanič award for diploma thesis entitled The application of electrochemical impedance spectroscopy to PEM fuel cell systems.

Damir Vrančić, Janko Petrovčič, Samo Krančan, Danfoss Trata: Silver and gold prize for HVAC electrical valve innovation, granted by the Chamber of Commerce and Industry of Slovenia.

Janez Brank, Award for the current achievements in the Information Society area

Vladimir Jovanovikj, Dušan Gabrijelčič, Tomaž Klobučar, Best paper award at SECUREWARE 2011, The Fifth International Conference on Emerging Security Information, Systems and Technologies, Nice – Saint Laurent du Var, france, August 21 – 27 2011.

**Bogdan Filipič**, **Miha Mlakar**, **Erik Dovgan**, **Tea Tušar**, Silver award for excellence of innovative industries at the 6th Slovenian Innovation Forum for Pedius, a system for computer-aided reconstruction of wall paintings, Ljubljana, 23. 11. 2011

**Tomaž Kompara**, Dean's praise for the best students in academic year 2010/2011, University of Ljubljana, Faculty of Electrical Engineering, Ljubljana, 29. 11. 2011

Damjan Kužnar, Matjaž Gams, Blaž Mahnič, Domen Marinčič, Rok Piltaver, TARAS Award at the 3rd Industrial Forum of Innovation, Portorož, R&D and Technology (IRT) for successful collaboration between research institution and industry, project »Intelligent Laboratory System for Healthcare (iLab)«, 6. 6. 2011

Andrej Prošek, Founding member recognition for the contribution in the establishment of the Nuclear Society of Slovenia, Ljubljana, Nuclear Society of Slovenia

Mitja Uršič, ENEN Prize, Nice, France, ENEN, Modeling of solidification effect in fuel coolant interactions



Presentation to the winners of the Jožef Stefan Golden Emblem Prize. From left to right: Prof. Jadran Lenarčič (Director of the JSI), Prof. Vanja Ambrožič (mentor, accepting the award on behalf of the winner Dr. Mitja Nemec), Dr. Petra Kocbek (winner), Dr. Miha Ravnik (winner) and Prof. Dragan D. Mihalović (President of JSI Scientific Council).

# **REVIEW OF PUBLICATIONS**

### FOR 2011

Department	Omiginal Antiplast	Deelve	Datant Appl and	Theorem
Department	Original Articles"	BOOKS	Patent Appl. and	Theses
Department of Theoretical Physics (F.1)	129		Grants	
Department of Low and Medium Energy Physics (F-2)	74	3	1	1
Department of Thin Films and Surfaces (F-3)	19	5	1	1
Department of Surface Engineering and Ontoelectronics (F-4)	78		3	1
Department of Solid State Physics (F-5)	191	5	5	
Department for Complex Matter (F-7)	61	3	6	3
Department of Reactor Physics (F-8)	83	2		2
Department of Experimental Particle Physics (F-9)	142	- 1		-
Department of Inorganic Chemistry and Technology (K-1)	34	2	3	
Department of Physical and Organic Chemistry (K-3)	20	2	1	
Electronic Ceramics Department (K-5)	68		1	1
Engineering Ceramics Department (K-6)	4		3	1
Department for Nanostructured Materials (K-7)	66		4	3
Department for Synthesis of Materials (K-8)	37	1	1	
Department for Advanced Materials (K-9)	44			1
Department of Biochemistry, Molecular and Structural Biology (B-1)	18	1		2
Department of Molecular and Biomedical sciences (B-2)	15			
Department of Biotechnology (B-3)	39	4	3	1
Department of Environmental Sciences (0-2)	108	17		3
Department of Automation, Biocybernetics and Robotics (E-1)	47	2		2
Department of Systems and Control (E-2)	54			3
Artificial Intelligence Laboratory (E-3)	36	4		2
Laboratory for Open Systems and Networks (E-5)	22			1
Department of Communication Systems (E-6)	62		1	2
Computer Systems Department (E-7)	26			
Department of Knowledge Technologies (E-8)	44	1		1
Department of Intelligent Systems (E-9)	65		1	
Department of Reactor Engineering (R-4)	64	2		2
Reactor Infrastructure Centre (RIC)	54	7		
Centre for Networking Infrastructure (CNI)	2			
Science Information Centre (SIC)	1			
Energy Efficiency Centre (EEC)	13	1		
Centre for Knowledge Transfer in Information Technologies (CT-3)	1	2		
Milan Čopič Nuclear Training Centre (ICJT)	3			
Radiation Protection Unit (SVPIS)	2			
Director's Office (U-1)	2			
Centre for Technology Transfer and Innovation (CTT)	1	1		
Jožef Stefan Institute	1730	62	33	33

\* 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 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.

## **R & D PROJECT PARTNERS**

- 1. ARAO-Agency for Radwaste Management, Ljubljana
- 2. Cinkarna Celje, d. d., celje
- 3. Časnik Finance, d. o. o., Ljubljana
- 4. Danfoss Trata, d. o. o., Ljubljana
- 5. Dentas, Maribor
- 6. Development Centre Novo mesto, d. o. o, Novo mesto
- 7. Domel, d. o. o., Železniki
- 8. Energetika Ljubljana, d. o. o., Ljubljana
- 9. Gen Energija, d. o. o., Krško
- 10. Geoplin Plinovodi d. o. o., Ljubljana
- 11. Gorenje Household Appliances, Velenje
- 12. Inea, d. o. o., Ljubljana
- 13. Intech Les, d. o. o., Unec
- 14. Kekon, d. o. o., Žužemberk
- 15. Knauf Insulation, d. o. o., Škofja Loka
- 16. Kolektor Group, d. o. o., Idrija
- 17. Lek, d. d., Ljubljana
- 18. Port of Koper, d. d., Koper

- 19. Magneti, Ljubljana, d. d., Ljubljana
- 20. Ministry of Defence of the Republic of Slovenia, Ljubljana
- 21. Ministry of Economic Development and Technology of the Republic of Slovenia, Ljubljana
- 22. Ministry of Health of the Republic of Slovenia, Ljubljana
- 23. Ministry of Higher Education, Science and Technology of the Republic of Slovenia, Ljubljana
- 24. Ministry of the Environment and Spatial Planning of the Republic of Slovenia, Ljubljana
- 25. Nuclear Power Plant Krško, d. o. o., Krško
- 26. RC eNeM Nano varistor, d. o. o., Ljubljana
- 27. RŽV, d. o. o., Gorenja vas
- 28. Siemens, d. o. o., Ljubljana
- 29. Telekom Slovenije, d. d., Ljubljana
- 30. Termoelektrarna Toplarna Ljubljana, d. o. o., Ljubljana
- 31. Thermal Power Plant Brestanica, d. o. o., Brestanica
- 32. Varsi, d. o. o., Ljubljana



# **INSTITUTE IN NUMBERS**

## 2010-2011



### REVENUES FROM OTHER ACTIVITIES $(\textcircled{\mbox{em}})$



### EMPLOYEES (FTE)



### REVENUES FROM PUBLIC SERVICES (€M)



### NUMBER OF PUBLICATIONS IN THE WEB OF SCIENCE



### NUMBER OF CITATIONS IN THE WEB OF SCIENCE



#### Annual Report 2011

# **RESEARCH DEPARTMENTS**

## DEPARTMENT OF THEORETICAL PHYSICS **F-1**

The research program of the Department of Theoretical Physics is focused on the theory of condensed-matter physics, statistical physics, the physics of nuclei, particles and fields, as well as biophysics and soft condensed-matter physics. The department also maintains its own highperformance computing facility, for which it develops the necessary software. These studies are carried out in close collaboration with several experimental groups at the Jožef Stefan Institute as well as with local and foreign universities and institutes. The department is also involved in various international projects.

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.

aces o

Head.

In a coupled-channel approach that incorporates quasi-bound quark-model states from the Cloudy Bag Model, Prof. Svjetlana Fajfer we have obtained a good overall agreement with the available experimental results for the partial widths of the S11 resonances, as well as for the pion, eta and kaon electro-production amplitudes. The results indicate that the N(1535) resonance is dominantly a genuine three-quark state rather than a quasi-bound state of mesons and baryons.

We simulated the scattering of two pions in chromodynamics on the lattice and determined the phase shift for elastic scattering in the channel with l=1. The phase shift has a resonance shape and we determined the mass and the width of the rho meson resonance, which agrees with the experiment. This presents the most accurate lattice QCD determination of mass and width among all hadronic resonances up to now. We calculated the observables related to the polarisation of the top quark in the process  $e^+e^- \rightarrow t$  bar t in the future linear collider.

The anomalous tW dj interactions, being a possible source of new effects in neutral B mesons oscillations, are investigated within a model indepen-

dent approach based on the assumptions of Minimal Flavor Violation. After that we extract preferred ranges of the anomalous tWdj couplings at the weak scale. These values are then compared to the previously considered

constraints coming from the rare radiative  $B \rightarrow Xs\gamma$  decay and the ones in the t  $\rightarrow$  bW decays. We find that the W helicity fractions can deviate by as much as 15% or 30% from their standard model values.

A model with scalar leptoquarks that couples to down quarks and charged leptons in neutral current processes, have been studied. We have overconstrained the couplings and found this model is able to explain the muon anomalous magnetic moment, whereas, at the same time, the tension between Vub and sin(2beta) CKM elements cannot be resolved. This model is a typical low-energy approximation of grand unified theories. In this context we have embarked on a study of proton stability when these and other leptoquarks are present. We have also studied an impact of meson mixing and electroweak precision data on the standard model with fourth generation.

A simple SM extension with only two new light fields – a scalar partner of the top (stop) (with a mass above m) and a light neutral fermion  $\chi^0$  (with a mass of a few GeV) - was analysed and coupled to the SM quarks via a Yukawa interaction. We showed that such a model can lead to a significant enhancement of the forward-backward asymmetry in t thar production at the Tevatron via the additional t that pairs produced from (stop anti-stop) decays. Then it was suggested that top physics could be studied at the LHCb experiment, and that the top production could be observed. Furthermore, we demonstrated that LHCb may be able to measure at bart production rate Figure 1: Three possible regimes of leptoquark couplings to muon that asymmetry, and thus indirectly probe an anomalous forward backward t bar resolve the muon anomalous magnetic puzzle

We have suggested that the top quark production and the decays at the LHC can offer a possibility to study new physics effects. We also used the first LHC data to set the limit on the scale of the left-right symmetry models of new physics.



t asymmetry in the forward region. Finally, we showed that the discovery channel for dark matter (DM) production at colliders could be through flavor violating interactions resulting in a novel signature of a single top and the large missing transverse energy. Several examples of the production of DM are dominated by the flavor violating couplings.

In our study we have derived bounds on the annual modulation of the dark matter signal in direct detection. It has been shown that it is possible to have a large enough direct CP violation in the SM to explain the latest data on charm decays. Flavor symmetric extensions of the standard model can explain the anomaly in the top-antitop production.

New data from the LHC was used to set an experimental limit on the scale of the left-right symmetry, i.e., on the masses of heavy right-handed gauge bosons and neutrinos, as well as on the scalar triplets that enter the seesaw mechanism. A potential discovery of a lepton number violating the signal at the LHC is directly connected to the neutrinoless double beta decay and other, lepton flavor violating, decays and therefore constitutes an interesting interplay between the high and low energy processes.

We studied the equations of gravity in the presence of a source, approximated as a point particle. We have shown that the dynamical variables of this system satisfy the constraints that, after a quantization, become a system of equations containing the Klein-Gordon, Wheeler-DeWitt and Schrödinger equations. We also explored a generalization of such a system to the 6-dimensional space, interpreted as a subspace of the 16-dimensional Clifford space.

#### Some outstanding publications in the past year

- Drobnak Jure, Fajfer Svjetlana, Kamenik Jernej. Interplay of t [to] bW decay and B[sub](d,s)-B[bar] [sub](d,s) mixing in minimal flavor violating models. *Phys. lett., Sect. B.* [Print ed.], 2011, vol. 701, no. 2, pp. 234-239.
- Tello Vladimir, Nemevšek Miha, Nesti Fabrizio, Senjanović Goran, Vissani Francesco. Left-right symmetry: from the LHC to neutrinoless double beta decay. *Phys. rev. lett.*, 2011, vol. 106, no. 15, pp. 151801-1-151801-4.

## The group of SOLID STATE THEORY AND STATISTICAL PHYSICS has been investigating the properties of novel materials with strongly correlated electrons, superconductors, nanosystems, ferroelectrics, as well as the properties of complex networks.

Within the theory of nonequilibrium phenomena in the systems with correlated electrons, we continued with the studies of different model systems driven by an electric field. Using recently developed numerical methods, we investigated the motion of a single-charge carrier, doped into the Mott insulator. We followed the time development of the system until reaching a stationary state. In this way we established several regimes, in particular the



Figure 2: Part of the studied social network MySpace: Users are represented by the nodes, while the links are the dialogs among them that are registered in a given time window. Colour and size of each node represent its topological 'importance' on the network.

adiabatic regime with Bloch oscillations and the dissipative regime with a steady current. In an analogous way we investigated the dynamics of a Holstein polaron in one dimension and a single hole in the two-dimensional t-J-Holstein model driven by a constant electric field. We also studied the anomalous behaviour of the driven integrable Mott insulator. It was shown that, at high temperatures, the field leads to a finite conductivity, whereby the weak-field limit indicates the existence of an ideal insulator, not conducting at any temperature. An analogous effect was found in the case of a weakly perturbed integrable system. With the method of exact diagonalisation we also calculated the variation of the spin stiffnes within the whole phase diagram of the anisotropic Heisenberg model.

In the framework of the theory of novel superconductors we have studied the behaviour of impurities (both nonmagnetic and magnetic) in contact with the Majorana edge states of chiral and helical topological superconductors. We have determined the spectral functions of anisotropic magnetic impurities on the surfaces of conventional superconductors. We have explored how the spin-orbit coupling affects the Kondo screening of a

magnetic moment. We used a particular model self-energy to describe the metallic phase of the overdoped cuprate superconductors and, with it, we successfully described several experiments, including angular dependent magneto-resistance, angular resolved photoemission and specific heat. We presented the results of our investigation of the correlated behaviour in transition-metal oxides. We demonstrated an agreement of our theoretical results on the correlated behaviour in  $Sr_2RuO_4$  with the experiment. We continued the investigation of transport properties of novel npictide superconductors using several-band phenomenological models. In collaboration with the experimental group we studied relaxor ferroelectrics in the framework of the Landau model. The temperature dependence of

the first Landau coefficient was derived from the spherical random bond–random field model of relaxors.

Continuing the research of quantum nanosytems we analysed two electrons with entangled spins. It was shown that such a case can be studied in ordinary 3D space, where the angles play the role of angular momenta. Similarly, one can represent the quantum entanglement within the framework of hidden variables. We worked on various problems related to transport properties of nanoscopic systems. We showed that, by utilizing the spin-Seebeck effect in quantum dots, one can effectively generate spin currents for spintronics applications. With the application of a previously developed numerical method, we followed the motion of a charge carrier, doped into the Mott insulator, and driven by a constant electric field. We established several regimes in the system, in particular the adiabatic regime with Bloch oscillations, and the dissipative one revealing a steady current.

Using the theory of complex systems and networks, we analyzed large datasets of user activity at Blogs and similar Web portals, where the interaction among the users is mediated by a text of messages. In combination with the machine learning methods of a text analysis, we determined the emotion contents of each message and studied how the emotion affects the collective behaviours of the users. Using numerical methods, we have studied the processes of colloidal aggregation in the presence of competing forces.

#### Some outstanding publications in the past year

- Žitko Rok, Lee Minchul, López Rosa, Aguado Ramón, Choi Mahn-Soo. Josephson current in strongly correlated double quantum dots. *Phys. rev. lett.*, 105 (2010) 116803.
- Mierzejewski Marcin, Vidmar Lev, Bonča Janez, Prelovšek Peter. Nonequilibrium quantum dynamics of a charge carrier doped into Mott insulator, coupled to phonons. *Phys. rev. lett.*, 106 (2011) 196401.

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

We studied the effects of the (quenched) disorder on the interactions between charged macromolecules. We generalized the Poisson-Boltzmann theory of macromolecular interactions to the case of polarizable ions and

complex media. We also proposed a theory of strong electrostatic coupling in multicomponent electrolyte solutions. In addition, we started working on the theory of ionic liquids. We investigated the ion distribution and overcharging on charged interfaces with dielectric inhomogeneities in the presence of asymmetric electrolytes containing polyvalent and monovalent ions. We formulated an effective "dressed counterion" approach and showed that it agrees with the results of the explicit Monte Carlo simulations.

Liquid crystalline phases made from bent-core molecules were studied both experimentally and theoretically. We focused on the orthogonal ferroelectric smectic phase, the ferroelectric phase with the highest symmetry observed so far. Using a discrete model, we analyzed the conditions needed for the formation and stabilization of the phases of the periods larger than 4 layers. We showed that the longest possible period has 6 layers, which has been confirmed experimentally. We developed a collection of demonstration liquid-crystal experiments that can be used at the introductory university and high-school levels. We also investigated optical properties of the nanocomposite materials made of cobalt nanoparticles dispersed in organic liquid host.

We proposed a continuum theory for the cluster formation in hard-core/ soft-shoulder colloids and we have shown that it reproduces the correct sequence of cluster morphologies. Using this theory, we also rederived the



Figure 3: Computer rendering of the cucumber mosaic virus capsid (strain FNY)

clustering criterion; this real-space derivation is more transparent than the existing inverse-space theories. We studied orientational ordering of the colloidal ionic molecules on periodic substrates, observing stable "supermolecules".

We explored their structural properties and the response to the external fields. Ordering and entropy-driven transport of colloids on soft substrates in gravitational field was also investigated.

We analyzed the problem of DNA condensation and electrostatic interactions in viruses. We also studied periodic bulk aggregates of lipid vesicles. We showed that the equilibrium shapes minimize the total edge length at a fixed volume and area, and that, at small reduced volumes, the stable shapes are We investigated the ion distribution and overcharging on charged interfaces with dielectric inhomogeneities in the presence of asymmetric electrolytes containing polyvalent and monovalent ions. oblate. We proposed a model of bacterial surface motility, which reproduces some of the experimentally observed properties. Using the maximum-entropy production principle, we studied the enzyme kinetics and we showed that in any internal enzyme transition, there is an extreme of entropy production with respect to the appropriate kinetic constant. With our theoretical studies of an aspirin-inducing asthmatic attack, we established a gene expression of enzymes in arachidonic acid metabolism as a reasonable explanation of the phenomenon, and it can be used to distinguish between different populations of asthmatics.

#### Some outstanding publications in the past year

- 1. Matthäus Franziska, Mommer Mario S., Curk Tine, Dobnikar Jure. On the origin and characteristics of noiseinduced Lévy Walks of E. Coli. *PLoS one*, 2011, vol. 6, no. 4, pp. e18623-1-e18623-8.
- Ben-Yaakov Dan, Andelman David, Podgornik Rudolf. Dielectric decrement as a source of ion-specific effects. J. chem. phys., 2011, vol. 134, str.074705-1-074705-12.

#### Organization of conferences, congress and meetings

- 1. The role of heavy fermions in fundamental physics, Portorož, Slovenia, 11.-14. 4. 2011
  - Understanding hadronic spectra, Bled, Slovenia, 4.–11. 7. 2011
- 3. Selected challenges in flavor physics, Medana, Slovenia, 15.-16. 9. 2011

## INTERNATIONAL PROJECTS

2.

Physics of Complex Colloids: Equlibrium and Driven Degrees of Freedom 1. COMPLOIDS BI-JP/11-13-003 7. FP. 234810 Prof. Takami Tohvama, Yukawa Institute for Theoretical Physics, Kvoto University, EC; Dr. Helmut Schaschl, University of Vienna, Research Services & International 2. Kyoto, Japan Prof. Janez Bonča Relations, Vienna, Austria Asst Prof Primož Ziherl Dr Jure Dobnikar 12. Theory of Materials for Spin Electronics and Dynamics of Magnetic Nanostructures 3. Low Dimensional Quantum Magnets for Thermal Management Joint Research Arrangement LOTHERM Dr. Michiyasu Mori, Japan Atomic Energy Agency (JAEA), Ibaraki, Japan 7. FP. 238475 Prof. Janez Bonča EC; Dr. Laura Hemker, Leibniz Institute for Solid State and Materials Research Dresden, 13. Hadron Structure in Chiral Quark Models vs. Lattice QCD Dresden, Germany BI-PL/10-11-018 Prof. Wojciech Broniowaski, H. Niewodniczanski, Institute of Nuclear Physics, Polish Prof. Peter Prelovšek 4. Collective Emotions in Cyberspace Academy of Science, Krakow, Poland CYBEREMOTIONS Prof. Bojan Golli, Prof. Simon Širca 7. FP. 231323 14. Self-Assembly in Ionic Liquids EC; Prof. Janusz Holyst, Warsaw University of Technology, Warsaw, Poland Research Sub-Contract Prof. Bosiljka Tadić Dr. Sue Cooper, University College London, Research Finance Administrator, Research 5. Physics of Competition and Conflicts Administration, London, Great Britain COST MP0801 Prof. Rudi Podgornik EC; COST Office, Brussels, Belgium 15. Correlated Electron Systems Coupled to Lattice Degrees of Freedom Prof. Bosiljka Tadić BI-US/11-12-015 Dr. Daniel Batista, Los Alamos National Laboratory, Los Alamos, NM, USA 6. Training in the Frame of the Leonardo da Vinci Mobility at the Foreign Institute - ISIT LDV-MOB-74/11, 2011-7933 Prof. Janez Bonča EC; CMEPIUS, Ljubljana, Slovenia 16. Interplay Between Precision Measurements and LHC Discoveries Dr. Miha Nemevšek BI-US/11-12-018 Aspects of Physics beyond the Standard Model and the Holographic Quantum Field Prof. Alexander Kagan, University of Cincinnati, Geology - Physics 400, Cincinnati, OH, Theory Gravity Correspodence USA BI-AR/09-11-006 Dr. Jernej Fesel Kamenik Prof. Adrián René Lugo, Instituto de Física de La Plata, Departamento de Física, 17. Supersymmetry and Grand Unification Universidad Nacional de La Plata, La Plata, Argentine BI-US/09-12-036 Dr. Stephen Barr, University of Delaware, Department of Physics and Astronomy, Prof. Borut Bajc Flavor of Physics at LHC and Super Flavor Factory 8 Newark, DE, USA PROTEUS 2010 - 2011 Prof. Borut Bajc BI-FR/10-11-PROTEUS-006 Dr. Emi Kou, Linear Accelerator Laboratory, Universite Paris-Sud 11, UMR 8607, Paris, France **R &D GRANTS AND CONTRACTS** Dr. Jure Dobnikar 9. Physics from the Grand Unification Scale to LHC Energies Carbon nanotube-based spin qubits PROTEUS 2010 - 2011 1. Prof. Anton Ramšak BI-FR/10-11-PROTEUS-014 2 Active devices - dispersion force based nanoactuators Dr. Stephane Lavignac, Institute of Theoretical Physics, CEA/Saclay, Gif-sur-Yvette, Prof. dr. Rudolf Podgornik France 3 Theory of thermal and spin transport in novel materials with correlated electrons Prof. Borut Bajc Prof Peter Prelovšek 10. Adhesion of Liposomes at Electrode 4 Superconductivity and magnetism in new iron-based superconductors BI-HR/10-11-010 Dr. Peter Jeglič Dr. Nadica Ivošević DeNardis, Ruđer Bošković Institute, Zagreb, Croatia 5 Non-equilibrium dynamics of interacting electron systems Asst. Prof. Primož Ziherl Prof. Peter Prelovšek 11. Theoretical Studies of Dynamical Properties in Correlated Electron Systems Coupled to External
Theoretical Aspects and Empirical Analysis of Labour Market Impact of Flexicurity 6. Dr. Tomaž Rejec

1. Katarina Susman, Pojem faznega prehoda pri pouku fizike (mentor Mojca Čepič).

prof. J. H. Jefferson, Oxford University and technology company QinetiQ, Great Malvern,

dr. Michael Fearn, Oxford University and QinetiQ, Great Malvern, Great Britain, 23.1.-

prof. dr. Marcin Mierzejewski, University of Katowice, Katowice, Poland, 10.-25. 2. 2011

Vincent Demery, Laboratoire de Physique Théorique, IRSAMC, Université Paul Sabatier,

Mathematics, Sarajevo, Bosnia and Herzegovina, 10.-13. 4. 2011 and 17.-24. 12. 2011

Fairfax, VA and National Institute of Standard and Technology, Gaithersburg, MD, USA,

prof. dr. Takami Tohyama, Yukawa Institute of Theoretical Physics, Kyoto University,

dr. Giuseppe Policastro, Ecole Normale Superieure, Paris, France, 24. 3. 2011

prof. dr. Qaisar Shafi, University of Delaware, Delaware, USA, 9.-15. 4. 2011

10. prof. dr. Gustavo Castelo Branco, Centro de Física Teórica de Partículas, Lisbona,

12. prof. dr. Ilja Doršner, University of Sarajevo, Institute of Natural Sciences and

14. dr. Indu Satija, Department of Physics and Astronomy, George Mason University,

dr. Paride Paradisi, Technische Universität München, Germany, 1.-15. 5. 2011
 dr. Mauricio Sturla, Universidad Nacional La Plata, Argentina, 4.-13. 5. 2011

20. dr. Giannis Georgiou, Technical University Vienna, Austria, 1.-10. 8. 2011 21. dr. Christopher Smith, Universite Lyon, Villeurbanne Cedex, France, 11.-15. 7. 2011

19. prof. dr. Giniyat Khaliullin, Max Planck Institute for Solid State Physics, Stuttgart,

13. dr. Stephane Lavignac, Saclay University, Paris, France, 10.-22. 4. 2011

15. prof. dr. Alex Kagan, University of Cincinnati, USA, 8.-15. 4. 2011 16. dr. Stefan Recksiegel, Technischen Universität München, Germany

dr. Robin Steinigeweg, Institut für Theoretische Physik, Technische Universität

- Single Magnetic Atoms and Magnetic Nanostructures on Metal Surfaces 7. Dr. Rok Žitko
- Synergies between precision measurements and LHC discoveries 8. Dr. Jernei Fesel Kamenik

VISITORS FROM ABROAD

Ai Sakashita, Ochanomizu University, Tokyo, Japan, 10.-19. 1. 2011

MENTORING

Great Britain, 11.-25. 1. 2011

Braunschweig, Germany, 9.-15. 1. 2011

Kyoto, Japan, 15.–19. 2. 2011 and 11.–15. 9. 2011

11. dr. Fabrizio Nesti, Ferrara University, Ferrara, Italy, 7. 4. 2011

Toulouse Cedex 4, France, 4. 4.-14. 6. 2011

Ph. D. Thesis

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and 11. 5.-4. 6. 2011

Portugal, 15.-18. 4. 2011

Germany, 9.-14. 6. 2011

## RESEARCH PROGRAMS

- Theory of condensed matter and statistical physics 1. Prof. Janez Bonča
- Theoretical physics of nuclei, particles and fields 2. Prof. Svjetlana Fajfer
- Biophysics of polymers, membranes, gels, colloids and cells 3. Prof. Rudolf Podgornik
- 22. dr. Takanori Sugimoto, Yukawa Institute of Theoretical Physics, University of Kyoto, Kyoto, Japan, 1. 6.-15. 7. 2011
- prof. dr. Stefan Thurner, Complex Systems Research Group, Medical University of Vienna, Vienna, Austria, 20.–23. 1. 2011
- 24. dr. Gerhard Kahl, Technical University Vienna, Austria, 9.-10. 8. 2011
- 25. dr. Nadica Ivošević DeNardis, dr. Amela Hozić Zimmerman, Ruđer Bošković Institute, Zagreb, Croatia, 13.-19. 11. 2011
- 26. prof. dr. Alejandra Melfo, Los Andes University, Merida, Venezuela, 28. 7. 2011
- prof. dr. Antun Balaž, Institute of Physics Belgrade, Serbia, 30. 9. 2011 28. prof. dr. Aharon Davison, Physics Department, Ben Gurion University, Beer Sheva, İsrael, 5.–9. 9. 2011
- 29. prof. dr. Tomonari Dotera, Kinki University, Osaka, Japan, 7.-11. 10. 2011
- 30. prof. dr. Masayuki Imai, Ochanomizu University, Tokyo, Japan, 18.-21. 10. 2011
- Sahib Babaee Tooski, Division of Theory of Solid State Physics, Institute of Molecular 31. Physics, Polish Academy of Sciences, Poznan, Poland, 5. 10.-31. 12. 2011
- 32. prof. dr. Bogdan R. Bulka, Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland, 23.–26. 10. 2011
- 33. dr. Oscar Cata, Departament de Física Teòrica, IFIC, Universitat de València CSIC, València, Spain, 14.-21. 9. 2011
- 34. dr. Marco Nardecchia, Centre for Particle Physics Phenomenology, CP3-Origins, University of Southern Denmark, Odense, Denmark, 20.-21. 10. 2011
- 35. prof. dr. Leszek Roszkowski, Sheffield University, Sheffield, Great Britain, 29. 9.-9. 10. 2011
- 36. dr. Marco Serone, SISSA, Trieste, Italy, 27. 10. 2011
- prof. dr. Blaženka Melić, Ruđer Bošković Institute, Zagreb, Croatia 2.11.-30.11. 2011 37.
- 38. prof. dr. Giorgio Pastore, Universita di Trieste, Trieste, Italy, 24.-25. 10. 2011
- 39. dr. Diego Aristizabal Sierra, IFPA, Department AGO, Universite de Liege, Liege, Belgium, 1.-16, 10, 2011
- 40. Soham Biswas, Calcuta University, Calcuta, India, 25.-30. 10. 2011
- 41. prof. dr. Branko Dragović, Institute of Physics Belgrade, Serbia, 20.-22. 11. 2011
- 42. dr. Frederica Lo Verso, Johannes Guttenberg University, Mainz, Germany, 18.-23. 5. 2011
- 43. dr. Michele Della Morte, Johannes Guttenberg University, Mainz, Germany, 18.-23. 5. 2011
- 44. dr. Ali Naji, School of Physics, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran, 2.-21. 11. 2011
- 45 dr. Milovan Šuvakov, Institute of Physics Belgrade, Serbia, 15.-25. 11. 2011
- 46. dr. Nataša Pržulj, Department of Computing, Imperial College London, Great Britain, 8.11.2011
- prof. dr. Veljko Zlatić, Institute of Physics, Zagreb, Croatia, 3. 10.-30. 12. 2011
- 48. dr. Luca Merlo, Technische Universität, München, Germany, 6.-7. 12. 2011
- 49. dr. Alvise Varagnolo, Universitat Autonoma de Barcelona, Spain, 29. 11.-3. 12. 2011

## **STAFF**

31. 5. 2011

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- 44. Luka Leskovec, B. Sc.
- 45. Anže Lošdorfer Božič, B. Sc.
- 46. Timon Mede, B. Sc.

# BIBLIOGRAPHY

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#### PUBLISHED CONFERENCE PAPERS

#### Invited Papers

- 1. Matej Pavšič, "On the Stueckelberg-like generalization of general relativity", In: *Proceedings of the IARD 2010, 7th Biennial Conference on Classical and Quantum Relativistic Dynamics of Particles and Fields, 30 May - 1 June 2010, Hualien, Taiwan,* (Journal of physics, Conference series, vol. 330, 2011), Bristol, Institute of Physics Publishing, 2011, vol.330, pp. 012011-1-012011-13, 2011.
- Bosiljka Tadić, Milovan Šuvakov, Gregor Trefalt, "Modelling structure of collodal assemblies: Methodology & examples", In: Proceedings of the 2011 International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE, June 26-30, 2011, Benidorm, Spain. Vol. 3, J. Vigo Aguiar, ed., [S. l.], CMMSE, 2011, pp. 1097-1103.
- 3. AUGER Collaboration: Darko Veberič et al. (504 authors), "The end of the cosmic ray spectrum", In: Papers presented at New Physics, complementarities between direct and indirect searches (LC10), (II Nuovo cimento C, vol. 34, no. 5, suppl. 1), LC10: New Physics: complementarities between direct and indirect searches, INFN-Laboratori Nazionali di Frascati, 30. nov. - 3. dec. 2010, Bologna, Italian Physical Society, 2011, vol. 34, suppl. 1, pp. 85-92, 2011.
- 4. Rok Žitko, "Magnetization curves for anisotropic magnetic impurities adsorbed on a normal metal substrate", In: *Physical properties of nanosystems: [proceedings of the NATO Advanced Research Workshop on Physical Properties of Nanosystems, Yalta, Ukraine, 28 September-2 October 2009]*, (NATO science for peace security series, B, Physics and biophysics), Janez Bonča, ed., Sergej Kručinin, ed., Dordrecht, Springer, NATO Public Diplomacy Division, cop. 2011, pp. 247-257.

#### Regular papers

1. AUGER Collaboration: Pedro Assis *et al.* (480 authors), "Multiple scattering measurement with laser events", In: *ECRS 2010*, (Astrophysics and space sciences transactions, vol. 7), Karl Scherer, ed., Göttingen, Copernicus, 2011, vol. 7, no. 3, pp. 383-386, 2011.

- AUGER Collaboration: Johannes Blümer *et al.* (470 authors), "Plans of the Pierre Auger Collaboration", In: *International Symposium on the Recent Progress of Ultra-High Energy Cosmic Ray Observation, Aichi, (Japan), 10-12 December 2010,* (AIP conference proceedings, vol. 1367), Hiroyuki Sagawa, ed., Melville, New York, American Institute of Physics, 2011, pp. 126-131.
- 3. Oliver Bodensiek, Rok Žitko, R. Peters, Thomas Pruschke, "Heavy fermions and superconductivity in the Kondo-lattice model with phonons", In: *Physical properties of nanosystems: [proceedings of the NATO Advanced Research Workshop on Physical Properties of Nanosystems, Yalta, Ukraine, 28 September-2 October 2009]*, (NATO science for peace security series, B, Physics and biophysics), Janez Bonča, ed., Sergej Kručinin, ed., Dordrecht, Springer, NATO Public Diplomacy Division, cop. 2011, pp. 233-246.
- AUGER Collaboration: Rossella Caruso *et al.* (480 authors), "General overview of recent results from the Pierre Auger Observatory", In: *ECRS 2010*, (Astrophysics and space sciences transactions, vol. 7), Karl Scherer, ed., Göttingen, Copernicus, 2011, vol. 7, no. 4, pp. 445-451, 2011.
- 5. Mojca Čepič, "Vsakodnevno življenje, naravoslovna metoda in fizikalne vsebine", In: Posvet o poučevanju fizike, kemije in matematike, SAZU, 22. septembra 2010, (Zbirka Znanje kot vrednota, 2), Mojca Čepič, ed., Ljubljana, Slovenska akademija znanosti in umetnosti, 2011, pp. 31-43.
- 6. Mojca Čepič, Jerneja Pavlin, "Lap-tops, mobiles, iPods and liquid crystals", In: *Conference proceedings*, 2nd World Conference on Technology and Engineering Education, Ljubljana, Slovenia, 5 - 8 September 2011, Zenon J. Pudlowski, ed., Slavko Kocijančič, ed., Melburne, World Institute for Engineering and Technology Education, WIETE, 2011, pp. 43-48.
- AUGER Collaboration: Bruce Dawson *et al.* (470 authors), "Highlights from the Pierre Auger Observatory", In: *International Symposium on the Recent Progress of Ultra-High Energy Cosmic Ray Observation, Aichi, (Japan), 10-12 December 2010,* (AIP conference proceedings, vol. 1367), Hiroyuki Sagawa, ed., Melville, New York, American Institute of Physics, 2011, pp. 11-16.
- AUGER Collaboration: Ralph Engel et al. (470 authors), "Some comments on the energy scale of the Pierre Auger Observatory", In: International Symposium on the Recent Progress of Ultra-High Energy Cosmic Ray Observation, Aichi, (Japan), 10-12 December 2010, (AIP conference proceedings, vol. 1367), Hiroyuki Sagawa, ed., Melville, New York, American Institute of Physics, 2011, pp. 50-53.
- 9. Fei Gao, Klemen Bergant, Tanja Bolte, Franco Coren, Tingyao He, Andrej Hrabar, Jurij Jerman, Ana Mladenovič, Samo Stanič, Janja Turšič, Darko Veberič, "Modelling, measurement and identification of Icelandic volcanic ash streaming over Slovenia", In: Proceedings of Earth observation for land-atmosphere interaction science, 3-5 November 2010, Frascati, Italy, (ESA SP, 688), Noordwijk, ESA Communications, cop. 2011, 7 pp.
- Bojan Golli, "Electroproduction of mesons in a chiral quark model", In: *Proceedings to the Mini-Workshop Understanding Hadronic Spectra, Bled, Slovenia, July 3-10, 2011*, (Blejske delavnice iz fizike, vol. 12, no. 1), Bojan Golli, ed., Mitja Rosina, ed., Simon Širca, ed., Ljubljana, DMFA - založništvo, 2011, vol. 12, no. 1, pp. 70-72, 2011.
- 11. AUGER Collaboration: M. Grigat *et al.* (480 authors), "Large scale anisotropy studies with the Pierre Auger Observatory", In: *ECRS 2010*, (Astrophysics and space sciences transactions, vol. 7), Karl Scherer, ed., Göttingen, Copernicus, 2011, vol. 7, no. 2, pp. 125-129, 2011.
- 12. Jernej Kamenik, "V<sub>ub</sub> and weak annihilation in inclusive semileptonic D/D<sub>s</sub> decays", In: Proceedings of the International Workshop on Charm Physics, Charm 2010, 21-24 October 2010, Beijing, China, (International journal of modern physic, B, vol. 2, 2011), Hai-Bo Li, ed., Singapore, World Scientific, 2011, vol. 2, pp. 78-82, 2011.
- 13. AUGER Collaboration: Matthias Kleifges *et al.* (480 authors), "The northern site of the Pierre Auger Observatory", In: *ECRS 2010*, (Astrophysics and space sciences transactions, vol. 7), Karl Scherer, ed., Göttingen, Copernicus, 2011, vol. 7, no. 3, pp. 319-325, 2011.
- 14. Nejc Košnik, Ilja Doršner, Jure Drobnak, Svjetlana Fajfer, Jernej Kamenik, "Scalar diquark in tī production and constraints on Yukawa sector of grand unified theories", In: Proceedings of the XXIst International Europhysics Conference on High Energy Physics, EPS-HEP2011, 21-27 July 2011, Grenoble, France, (Pos proceedings of science, vol. 2011, no. 380, 2011), Trieste, Sissa, 2011, vol. 2011, no. 380, pp. 1-6, 2011.
- 15. Maja Küčan, Milan Brumen, Marjan Skalicky, Mateja Lorber, "Pojasnjevalna vloga medicinske sestre pri seznanjanju preiskovanca z gastroendoskopsko preiskavo", In: Razvijanje medpoklicnega sodelovanja v času študija na področju zdravstvenih ved: zbornik

*predavanj z recenzijo*, Milica Lahe, ed., Aleksandra Lovrenčič, ed., V Mariboru, Fakulteta za zdravstvene vede, 2011, pp. 146-153.

- 16. AUGER Collaboration: A. Letessier-Selvon *et al.* (470 authors), "Anisotropy studies with the Pierre Auger surface array data", In: *International Symposium on the Recent Progress of Ultra-High Energy Cosmic Ray Observation, Aichi, (Japan), 10-12 December 2010,* (AIP conference proceedings, vol. 1367), Hiroyuki Sagawa, ed., Melville, New York, American Institute of Physics, 2011, pp. 94-99.
- 17. AUGER Collaboration: C. Meurer *et al.* (480 authors), "Heat: a low energy enhancement of the Pierre Auger Observatory", In: *ECRS 2010*, (Astrophysics and space sciences transactions, vol. 7), Karl Scherer, ed., Göttingen, Copernicus, 2011, vol. 7, no. 2, pp. 183-186, 2011.
- AUGER Collaboration: Petr Nečesal et al. (483 authors), "The fluorescence detector of the Pierre Auger Observatory", In: XIV International Conference on Calorimetry in High Energy Physics (CALOR 2010), 10-14 May 2010, Beijing, China, (Journal of physics, Vol. 293), Bristol, IOP Publishing, 2011, vol. 293, no. 1, 6 pp., 2011.
- 19. AUGER Collaboration: Thomas Paul *et al.* (469 authors), "Results from the Pierre Auger Observatory", In: *Proceedings of the 3rd International Conference on Time and Matter, 4-8 October 2010, Budva, Montenegro,* Martin O'Loughlin, ed., Samo Stanič, ed., Darko Veberič, ed., Nova Gorica, University, 2011, pp. 70-84.
- Saša Prelovšek, Christian B. Lang, Daniel Mohler, "Scattering phase shift and resonance properties", In: *Proceedings to the Mini-Workshop Understanding Hadronic Spectra, Bled, Slovenia, July 3-10, 2011*, (Blejske delavnice iz fizike, vol. 12, no. 1), Bojan Golli, ed., Mitja Rosina, ed., Simon Širca, ed., Ljubljana, DMFA - založništvo, 2011, vol. 12, no. 1, pp. 73-81, 2011.
- 21. AUGER Collaboration: G. Rodriguez *et al.* (480 authors), "Results from the Pierre Auger Observatory", In: *Proceedings of the 40th International Symposium on Multiparticle Dynamics*, Nick Van Remortel, ed., Pierre Van Mechelen, ed., Antwerp, Uitgeverij UPA University Press, cop. 2011, pp. 239-244.
- 22. Brigita Rožič, Zdravko Kutnjak, George Cordoyiannis, Boštjan Zalar, Slobodan Žumer, Simon Krause, Heino Finkelmann, Barbara Malič, Alja Kupec, Janez Holc, Marija Kosec, Raša Pirc, Robert Blinc, Marko Jagodič, Sašo Gyergyek, Mihael Drofenik, Samo Kralj, Gojmir Lahajnar, Zvonko Jagličić, "Liquid crystal elastomers, electrocalorics, and new soft magnetoelectrics: materials for advanced technologies", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 199-205.
- 23. Katarina Susman, Jerneja Pavlin, Saša Ziherl, Maja Pečar, Mojca Čepič, "Phase transitions in the frame of mechanical model", In: *Conference proceedings*, 2nd World Conference on Technology and Engineering Education, Ljubljana, Slovenia, 5 - 8 September 2011, Zenon J. Pudlowski, ed., Slavko Kocijančič, ed., Melburne, World Institute for Engineering and Technology Education, WIETE, 2011, pp. 38-41.
- Simon Širca, Bojan Golli, Manuel Fiolhais, P. Alberto, "Pion scattering and electro-production on nucleons in the resonance region in chiral quark models", In: *Hadron2011: proceedings of the XIV. International Conference on Hadron Spectroscopy, 13-17 June 2011, Munich, Germany,* B. Grube, ed., S. Paul, ed., N. Brambilla, ed., München, Technische Universität, 2011, pp. 520-524.
- 25. Gregor Trefalt, Barbara Malič, Bosiljka Tadić, Janez Holc, Danjela Kuščer, Marija Kosec, "Innovative approach to synthesis of Pb(Mg<sub>1/3</sub>(Nb<sub>2/3</sub>O<sub>3</sub> based materials using colloidal interactions", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 206-211.
- 26. AUGER Collaboration: Michael Unger et al. (470 authors), "Analysis of longitudinal air shower profiles measured by the Pierre Auger Observatory", In: International Symposium on the Recent Progress of Ultra-High Energy Cosmic Ray Observation, Aichi, (Japan), 10-12 December 2010, (AIP conference proceedings, vol. 1367), Hiroyuki Sagawa, ed., Melville, New York, American Institute of Physics, 2011, pp. 106-109.
- 27. Lev Vidmar, Janez Bonča, "Interplay between strong correlations and electron-phonon coupling in cuprates: comparison between different models", In: *Proceedings of the 15th Fifteenth Training Course in the Physics of Strongly Correlated Systems*, 4-15 October 2010, Vietri sul

Mare, Salerno, Italy, (AIP conference proceedings, vol. 1419, 2011), Adolfo Avella, ed., Ferdinando Mancini, ed., New York, American Institute of Physics, 2011, vol. 1419, pp. 271-275, 2011.

#### THESES

- B. Sc. Theses
  - 1. Urška Jelerčič, *Model of composite contact of two-component membranes:* undergraduate thesis, Ljubljana, [U. Jelerčič], 2011.
- Ambrož Kregar, *The influence of Rashba coupling on Wigner rotator:* undergraduate thesis, Ljubljana, [A. Kregar], 2011.
   Zala Lenarčič, *Dielectric breakdown in Mott insulator:* undergraduate
- thesis, Ljubljana, [Z. Lenarčič], 2011.
  Luka Leskovec, Pion and kaon scattering in lattice chromodynamics:
- undergraduate thesis, Ljubljana, [L. Leskovec], 2011.

# DEPARTMENT OF LOW AND MEDIUM ENERGY PHYSICS

# **F-**2

Work in the low-energy physics of the F-2 department was mainly driven by the research programme "Study of atoms, molecules and structures with photons and particles" (P1-0112), the two projects that are running within the frame of the Slovenian Fusion Association (EUROATOM-MHEST) and international projects assigned to us as a member of the European network of ion-accelerator facilities SPIRIT. The basic and applied research was executed at home, mainly at the Microanalytical Infrastructure Center (MIC), and abroad, most frequently at the synchrotron laboratories around Europe (Elettra, ESRF, Soleil, Hasylab), where we have conducted research on the projects proposed by ourselves or in the frame of our collaborations.

We have continued with our studies of quantum interference of the indistinguishable electron pairs emitted by atoms in the course of photoabsorption or inelastic electron scattering. At GasPhase beamline at Elettra we have measured the angular distribution of  $(\gamma, 2e)$  reaction on the Ar 2p subshell and in collaboration with a group from the Miskolc University (Hungary) we continued to study the interference effects in the electron impact induced Head: resonant Auger decay. We have, experimentally and theoretically, studied the decay of the He singly excited state in Asst. Prof. Matej Lipoglavšek a nonzero external DC electric field. Due to a large asymmetry of the probability for creating a singlet or a triplet metastable state, it turned out that the measurement of the metastable atomic yield as a function of the electric field strength represents a sensitive tool for studying the evolution of the Stark diagrams that becomes particularly complicated when large angular momentum states with non-negligible spin-orbit interactions are involved. In the field selected avoided crossing points we have stimulated an emission into the selected low lying final state using the Ti-Sapphire laser to gather more information about the nature of critical points. In collaboration with the research group from the LCPMR Laboratory at Universite P&M Curie in Paris, we detected a magnetic bottle signal of the double inner shell ionization in simple organic molecules. Since the synchrotron light has too small

an intensity for the multiphoton absorption to be important, these events occur solely due to electron correlations. It turns out that the probability to form an additional hole at the same C atom in a C<sub>2</sub>H<sub>2</sub> molecule is about one thousand times lower (Phys. Rev. Lett., 106, 063003), and if the hole is on the other C atom of the molecule, it is a hundred thousand times lower than the probability to form a single K hole by photoabsorption (Phys. Rev. Lett., 107, 193004). The model calculations predict that the chemical sensitivity of a double photoionization, especially when two different atomic sites are involved, is larger than the sensitivity based on the single photoionization spectral shifts (ESCA).

In 2011, the JSI high-resolution X-ray spectrometer was employed in two experimental projects on the ID26 beamline at the ESRF synchrotron in Grenoble. The first, performed in collaboration with British researchers from the University of Sheffield, involved high resolution XES measurements to study the local chemical environment of S and Cl in a series of glasses used for the vitrification of the high-level radioactive waste. Vitrification is a technology for the immobilisation of the high-level radioactive waste, preventing a release of radionuclides to the environment during a deep geological repository. The ionizing radiation, emitted by the radioactive wastes, interacts with the vitreous material leading, potentially, to long-term changes of the physical and chemical properties of the material. From our measurements we could determine the oxidation state and the environment of sulphur within the glasses and also the relative amount of the reduced sulfur in the  $\gamma$ -irradiated samples as a function of the absorbed dose. The second experimental project at the ESRF was dedicated to the study of structural and dynamical properties of chlorinated hydrocarbons (HCC) in the gaseous state. The high resolution X-ray absorption (XAS) and resonant inelastic X-ray scattering (RIXS) spectra at the Cl K edge were collected for





Figure 1: (a) Histogram of the sum of the energies of 2 photoelectrons associated with the core DI in  $C_2H_2$  at the photon energy of 770.5 eV when detected in coincidence with the two released Auger electrons of 200-270 and 270-320 eV. (b) Ab-initio model result. (c) Same as in (a) but the coincidence is with only one Auger electron of 230-250 eV. Vertical bars at the bottom correspond to our theoretical calculations for the position of the DCH main lines (Phys. Rev. Lett., 107, 193004, 2011).

eleven HCC gaseous targets (3 chloromethanes, 4 chloroethanes, 3 chloroethenes, and a chlorobenzene). The overall energy resolution of our resonant measurements ( $\sim 0.5 \text{ eV}$ ) was below the lifetime broadening of the Cl 1s hole yielding the possibility for a very detailed structural analysis of the studied HCC molecules. Using the core-hole clock method, the fast nuclear dynamics, induced by the Cl 1s excitation, can also be studied on the  $\sim 1$  fs timescale



Figure 2: Experimental spectrum of a two-electron-one-photon (TEOP)  $(1s^{-2})^{1}S_{0} \rightarrow (2s^{-2}P^{-1})^{1}P_{1}$  transition in doubly ionized Mg (Phys. Rev. Lett. 107, 053001, 2011).

given by the Cl 1s core-hole lifetime. In collaboration with the group from the University of Fribourg we published, in 2011, the first experimental evidence for the correlated two-electron one-photon (TEOP) transitions following a single-photon K-shell double ionization (Phys. Rev. Lett. 107, 053001). The measurements on solid Mg, Al, and Si targets were performed and the TEOP transition energies and the branching ratios relative to the radiative oneelectron hypersatellite transitions were determined. In collaboration with Fribourg, the high resolution KMM radiative Auger X-ray spectra of solid Ca induced by monochromatic synchrotron radiation (Phys. Rev. A 83, 042513), and the electron-induced  $L_{s}M$  two-step double ionization cross-sections of metallic Pd (Phys. Rev. A 83, 022708) were published, respectively. In collaboration with the French colleagues from the UPMC in Paris we published our measurements of the resonant inelastic X-ray scattering (RIXS) spectra of the CH<sub>3</sub>I molecule near the iodine L<sub>2</sub> and L<sub>3</sub> absorption edges (J. Chem. Phys. 134, 144308). The measured spectra reveal fingerprints of ultrashort dissociation of the molecule on the timescale of  $\sim 200$  attoseconds given by the iodine L-shell core-hole lifetime. The high-resolution X-ray spectroscopy

was successfully applied also in the proton-induced X-ray measurements (HR-PIXE) at the IJS Microanalytical center. Within 2011, the measurements of crossover (K $\beta$ ") and valence (K $\beta_{2,5}$ ) transition in the proton-induced X-ray spectra of chromium oxides were published (*Spectrochimica Acta* B66, 461-469). The parametrization of these contributions as a function of chemical and structural properties was performed for 3d metal compounds yielding a possibility for their chemical and structural speciation (*J. Anal. At. Spectrom.* 26, 2467). The high-resolution X-ray spectroscopy was also applied to improve detection limits of the X-ray analysis (PIXE and XRF methods) in the case of trace elements with the atomic number in the close vicinity to the atomic number of the target matrix element (*X-Ray Spectrom.* 40, 2).

In collaboration with the Centre of excellence CO NOT a series of *in-situ* experiments for XANES and EXAFS on Li-ion and Na-ion batteries were performed, with several nanostructured cathode materials (NaVPO<sub>4</sub>F, Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>3</sub>, Li<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>4</sub>, Li<sub>2</sub>Mn<sub>0.2</sub>Fe<sub>0.8</sub>PO<sub>4</sub>, Li<sub>2</sub>Mn<sub>0.5</sub>Fe<sub>0.5</sub>PO<sub>4</sub>) and Li-sulfides. The XAS spectra were recorded during the reduction



Figure 3: Comparison of the Cd L edges in vapour and metal (Phys. Rev. A 84, 052508, 2011). The vapour attenuation is renormalized to the value of the metal at both extreme ends of the measured interval. A, continuum threshold in metal; B, edge resonance in vapour; C, atomic threshold derived from the experiment (see the text), and D, NIST atomic threshold value.

and oxidation of the materials with the C/15 dynamics and during heating in air up to 400°C. We registered the change of valence of V, Mn and Fe during the processes, providing the key information on the battery dynamics and opening the way to optimization of the synthesis of the material with the maximum capacity. Another long-term project, in collaboration with the National Institute of Chemistry, involves the XAS measurements on the catalytic mesoporous molecular sieves doped with Ca, Cr, Mn, Fe, Ni and Cu, containing also organic building units. The valence of dopants and their atomic neighbourhood is determined, to elucidate their catalytic properties. The materials are aimed at commercial applications such as molecular sieves and separators, adsorbents and ion traps, as well as solid heterogeneous catalysts sensitive to the molecular shape (N. Novak Tušar et al., Adv. funct. mater., online). In collaboration with the Biotechnical Faculty of the University of Ljubljana, we performed two series of XAS experiments to determine the distribution of Cd in the cells of Cd-hyperaccumulating plants (Thlaspi *praecox*) and to determine the Cd binding at the cellular and tissue levels. The submicron monochromatic X-ray beam of the lateral resolution of 0.2 micrometers was used. The distribution of sulphur, chlorine and zinc was scanned simultaneously, to reveal correlations between the elements. At several points, the XANES spectra of Cd L<sub>2</sub> and S K edges were measured to establish the binding of Cd and the role of the sulphur in it. The transport of the metal from the roots to the stems, leaves and other tissues should be

elucidated, together with the molecular and cellular mechanisms that induce the tolerance to the noxious Cd cations. In collaboration with the Laboratory for Material Research of the University of Nova Gorica we analysed the doping site of Mn in the crystal structure of Sr titanate and of Fe in Ba titanate, to explain the anomalous magnetic proper-

ties of the materials. The data of high-resolution L-region absorption spectra of monoatomic vapour of Cd and of Ba ion in an aqueous solution were analysed and published (*Phys. Rev.* A 84, 052508). New details of multielectron excitations in the elements, and of the L-shell collective excitations in general were established. Summarily, our

XAS-based research led to the publication of 8 scientific articles in high-IF

international journals in 2011.

The work was continued on the project no. 1.4.1 "Processes with neutral hydrogen atoms and molecules" of the Slovenian Fusion Association (SFA -Association EURATOM-MHEST). The study of the influence of the radiation damage in tungsten on hydrogen retention has been initiated. Tungsten is the material of choice for key components in fusion reactor due to its thermal properties and low hydrogen retention under normal conditions. The later property is particularly important due to the safety restrictions on the total amount of retained tritium, a heavy and radioactive hydrogen isotope, which is the fusion fuel in the reactor. Radiative damage in the materials will normally occur during the operation of a fusion reactor due to the exposure to the high-energy neutrons (14.1 MeV) which are the product of the main fusion reaction (D+T $\rightarrow$  4He+n). We are studying hydrogen retention in tungsten exposed to the neutral lighter hydrogen isotopes (H and D atoms) by using the methods with fast ion beams (ERDA, RBS and NRA). The experiments are performed with the reference undamaged, ITER grade, samples and damaged samples, generated by the exposure to high-energy tungsten ions of the appropriate total flux. The damage generated in this way has similar



Figure 4: Measured distribution of vibrational states of deuterium molecules created by atom recombination on tungsten and copper ((S. Markelj and I. Čadež, J. Chem. Phys. 134, 124707, 2011). For the  $H_2$  molecule the corresponding vibrational temperatures are:  $T_v$ =2700 K (Cu) and  $T_v$ =3700 K (W).

properties as the damage induced by an exposure to high-energy neutrons. Work on this subject is performed in tight collaboration with the Max-Planck Institute for Plasma Physics (IPP) in Garching, Germany, and is included in the work program of the EFDA (European Fusion Development Agreement) as a project of the EU Task Force for Plasma-Wall Interaction (TF PWI), "Hydrogen recycling on irradiated tungsten" (WP11-PWI-01-02-03/MHEST/ BS). Within the same project of the SFA we have finalised the evaluation of the vibrational excitation of hydrogen molecules (H<sub>2</sub> and D<sub>2</sub>) produced by an atom recombination on tungsten and copper in a special cell with partially dissociated gas (*J. Chem. Phys.* 134, 124707). Dissociative electron attachment (e+AB $\rightarrow$ A+B-, B being H or D) has also been studied in H<sub>2</sub>, D<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub> in C<sub>3</sub>H<sub>8</sub> and new data on cross-sections have been obtained. This is important not only for the edge plasma in fusion reactors but also for astrophysics (*Phys. Rev. Lett.*, 106, 243201). With these measurements we have actively participated in the COST action CM0805 – "Chemical cosmos: Understanding the Chemistry in Astronomical environments".

Within our collaboration with the ALOISA beamline group at the Elettra synchrotron (Laboratorio TASC IOM-CNR, Trieste, Italy) we studied the ordering and electronic properties of the nanostructured and hybrid organic interfaces. In our study of the hetero-organic self-assemblies of Benzoic acid (BA) on the vacuum deposited cysteammine (CA) monolayer on the Au substrate we showed that the intermolecular NH<sub>2</sub>-COOH recognition scheme and the specific coupling via the hydrogen bond formation produces an ordered self-assembled hybrid structure (SAM-on-SAM). Based on its chemical recognition and molecular ordering nature, the BA-CA hybrid assembly is a promising candidate for a parallel fabrication of the hierarchically assembled nanodevices out of the functionalized building blocks (*J. Phys. Chem. Lett.*, 2, 3124.) In our study of the amine terminated organic molecules on an Au substrate (Tetramethyl-Benzenediammine, TMBDA) we evidenced the role of molecular coupling on its preferentiall adsorption and electronic structure at the hybrid interface. We found that the TMBDA molecules preferentially bind to the low coordinated Au sites through a nitrogen lone pair, which leads to an energy shift of the highest occupied molecular orbitals (HOMO). Our results show that, even though weak, the N-Au coupling can affect the electronic and transport properties across the hybrid molecular junction (*J. Phys. Chem. C, Nanomaterials and interfaces* 115, 12625.)

We studied the properties of different materials by measuring their hyperfine magnetic and electric fields with Mössbauer spectroscopy. Our research was focused on the properties of magnetic nanoparticles and cathode materials for lithium batteries. The Mössbauer spectroscopy studies of superparamagnetic Ba-hexaferrite nanoparticles prepared by a modified hydrothermal synthesis showed a decrease in the nanoparticle magnetization with respect to the bulk magnetization, a consequence of different distributions of iron atoms over the  $4f_1$ ,  $4f_2$ , 2a, and 4b sublattices in nanoparticles. The broadened spectrum and the lower internal magnetic fields are therefore explained by a relatively large contribution of the near-surface Fe atoms in the nanoparticles compared to the contribution of the Fe atoms inside a particle (*Mater. Chem. Phys.* 127, 415). Several samples of pure Li<sub>2</sub>FeSiO<sub>4</sub> polymorphs, prepared by a hydrothermal synthesis and then quenched from either 400°C (Pmn2<sub>1</sub>), 700°C (P2<sub>1</sub>/n), or 900°C (Pmnb), were thoroughly investigated by Mössbauer spectroscopy. <sup>57</sup>Fe Mössbauer experiments showed that (i) iron in all

the polymorphs existed in the divalent oxidation state, and (ii) the chemical shifts and quadrupolar splittings are well correlated with the Fe–O bond lengths. An analysis of the isotropic NMR shifts of <sup>6</sup>Li nuclei revealed that they comprise two contributions of a comparable magnitude, a hyperfine (contact) shift and a pseudo-contact shift. Based on the structural models of  $\text{Li}_2\text{FeSiO}_4$ , both contributions could be successfully predicted by the first-principles calculations. The contact shift was obtained from the hyperfine-coupling constant on the <sup>6</sup>Li nuclei, which was calculated within a DFT/PAW approach, and the pseudo-contact shift was derived from the electron–nucleus dipolar matrix and the *g*-tensor, which was computed within the DFT/GIPAW frame (*Chem. Mater.* 23, 2735).

Intensive research with ion beams was carried out in 2011 at the ion accelerator Tandetron. Part of the efforts was devoted to the development of spectroscopic techniques, where we merged the existing knowledge on the interaction of fast ions with matter and the technical skills in the construction of detector systems based on our own design and production in the Institute's workshop. In 2011, we completed the construction of a cryostat and the accompanying equipment for the micro-PIXE spectroscopy on slices of biological tissue in a frozen hydrated state. With this step, we became the world's only laboratory that enables users to perform the element quantitative micro-PIXE analysis on thin slices of tissue in frozen hydrated state. In the frame of the EU 7FP project SPIRIT we carried out the construction of a spectrometer for MeV SIMS based on Time-Of-Flight principle. This will be installed at the ion microprobe and will allow measurements of the distribution of heavy molecules in biological tissue. Intense research work was devoted to the upgrade of two-dimensionally sensitive micro-PIXE method in a full three-dimensional tomography technique with a use of the X-ray lenses (*Nucl. Instr. Meth. B* 269, 2237). We developed a calculation algorithm, which allows a reconstruction of surface topography with a pair of simultaneously



*Figure 5: Archetypal SAM-on-SAM via the NH*<sub>2</sub>*-COOH molecular anchoring: benzoic acid/cysteammine/Au (J. Phys. Chem. Lett., 2, 3124, 2011).* 

acquired PIXE spectra by two spatially dislocated X-ray detectors. We assigned the name stereo-PIXE to the method based on its analogue in the optics with visible light. Within the fusion project in the EU 70P EURATOM programme we upgraded the micro-NRA method with the application of a thick-silicon detector for a total collection of fast protons from the reaction (3He,p) on light elements for the analytical work on the wall materials from the fusion reactors. Micro-PIXE was applied in a series of projects in the fields of biology, nanotoxicology and ecology, where we measured elemental distributions in the tissue sections prepared with shock-freezing and freeze-drying. The tissue preparation was carried out at the Biotechnical Faculty, University of Ljubljana. In collaboration with Université Catholique de Louvain, Belgium, we investigated the uptake of Zn in Cd in the plant Zygophyllum fabago, which exhibits promising potentials in the phytoremediation of the sites polluted with heavy metals. In collaboration with the Biotechnical Faculty, the University of Ljubljana, we investigated the effects of the biofortification on the iron uptake in wheat. We determined the distribution of iron in the grains and demonstrated the correlation between the iron concentration in the soil, wheat genotype and the concentration of iron in the wheat grain. The micro-PIXE method was effectively used in the field of nanotoxicology

for the research of the uptake of titanium oxide in the nanoform (S. Novak, D. Drobne et al., accepted for publication in *Environmental Toxicology and Chemistry*), silver and cobalt nanoparticles in the organism of *Porcellio Scaber*. We investigated the properties of thin films with the combined RBS/ERDA method in collaboration with the Department for Thin Films and Surfaces at the JSI, with the Ruđer Bošković Institute, Zagreb, Croatia and with the University of Leoben, Austria. Work was devoted to the hydrogen concentrations in the diamond-like carbon thin films (Čekada et al., accept. for publ. in *Surf. Coat. Technol.*). The ion accelerator laboratory is a Transnational Access (TNA) provider in the frame of the EU 70P SPIRIT. The programme enables access to the researchers from the European research area, based on a peer-reviewed project application. In 2011 we carried out six projects involving researchers from Belgium, Serbia, Spain, Hungary and Portugal.

In the frame of the collaboration between our XRF laboratory and the Biotechnical Faculty of the University of Ljubljana an analysis of the bulk plant materials have been performed in order to determine the average concentrations of elements, especially metals. The same material was then used to determine the concentrations of the elements at the organ and cellular levels by employing the microPIXE technique at the IJS's Tandetron accelerator (the SPIRIT programme) and also during a few experimental cycles at the synchrotron Elettra in Trieste and the ESFR in Grenoble. The work on the synchrotron facilities was also devoted to the development of the quantification of the intensity maps measured for different elements. Using the additional measurements of the absorption of the primary excitation beam in each measured point or pixel by a CCD camera or a photodiode, an evaluation of elemental concentrations in each pixel as well as the respective area weight and the absorption parameter of the residual matrix was possible. In 2011 the measurements at the IR spectromicroscopy beamline (SISSI) at the synchrotron

Elettra (Trieste) were devoted to studying the profile changes in the organic molecules in the plants treated with the nanoparticles of CuO. The measurements of the distribution of Na in the tissues of different genotypes of the tomato plants, resistant to salinity, were carried out at the TwinMic beamline in collaboration with »Groupe de Reserche en Physiologie végétale (GRPV) from Université Catholique de Louvain, Belgium. The measurements at the ID-21

beamline (XRF spectroscopy) at the ESFR in Grenoble were carried out within the framework of the project »Sub-cellular localisation of Cd in plant tissues« in collaboration with the Biotechnical Faculty, the University of Ljubljana. The objective of both projects was also the testing of the quantification software for elemental distribution in biological tissues, developed by Peter Kump. On the basis of the measured coherent and incoherent scattered radiation of the primary excitation beam in the XRF experiment, a methodology to determine the sort of plastic material was developed. The measurements of different food products with the objective to determine the mineral composition was carried out within the CRP project V4-1047, again in collaboration with the Biotechnical Faculty, the University of Ljubljana.

In the field of application of the ion beam analysis in archaeometry we mainly analysed glass. Using the methods of PIXE-PIGE we analysed a series of Roman glasses from Serbia and a series of Roman glasses from Albania. As a collaboration project with the IAEA we studied prehistoric, Roman and early medieval glass from Bulgaria, though the measurements have not been completed yet, as the light elements still have to be measured with the PIGE method. Tentatively, we measured the light elements with the microbeam Figure 6: Quantitative elemental distribution in wheat grain, obtained in vacuum and with the external beam in helium atmosphere. The quantification of these measurements is presently tedious, as we do not know well the spectral background and the detector efficiency in this region. As a new theme we started an analysis of the glass from the end of the 19th/beginning of the 20th centuries, which was pigmented by an addition of uranium. At the synchrotron Elettra we studied the degradation of textiles using the method of FTIR. In the field of experimental archaeology we made ballistic experiments with sling projectiles and applied statistical methods for classification of the lead acorns from the Slovenian sites.

In the A1 Collaboration at MAMI (Mainz, Germany) we have continued with a series of measurements with the new KAOS spectrometer, which allows the detection of positively and negatively charged reaction products up to the momenta of 1.5 GeV/c. We have constructed the aerogel Cherenkov counter employing an aerogel radiator with a refraction index of 1.055. The KAOS spectrometer is now fully instrumented on both the electron and the hadron arm. We have performed several calibration measurements of the electroproduction of the charged kaons and of the formation of hyperons in nuclei, as well as kaon electroproduction on proton targets: in these measurements, the electron spectrometer was raised out of the scattering plane, allowing for the extraction of the previously undetermined fifth-structure function. We have continued the data analysis of the high-precision double-polarization measurement of the electroproduction of the neutral pions on protons in the region of the Roper resonance. The final goals of the analysis are the recoil proton polarization components. We have published the results of a precision experiment, in which we searched for hypothetical light bosons mediating the interactions of the dark matter. There is also an ongoing effort of studying the virtual Compton scattering, aiming at determining the generalized polarizabilities as functions of the momentum transfer.

In the framework of the Hall A Collaboration at the Jefferson Laboratory we have performed two sets of measurements. We have collaborated in the run group of the E08-008, E08-010 and E07-006 experiments devoted to the studies of short-range correlations (SRC). We have also collaborated on the preparation of the experiments E08-007 and E08-027 in which we will investigate the elastic form-factors of a proton and the polarized structure function g2p.

In collaboration with the Department of Theoretical Physics at the JSI and the University of Coimbra, we continued our investigations of dynamical (electromagnetic and weak) processes on protons and neutrons in the energy region of the Roper resonance and of the negative-parity resonances. After having obtained excellent results for the electroproduction amplitudes, we are now extending our work to the corresponding weak amplitudes.

Members of the Infrastructure Group for Ionizing Radiation Measurements conducted a scientific research in connection with the Programmes P1-0102 and P1-0112, on the projects "Quality and genuineness of honey on the Slovenian market", and "Natural and anthropogenic gamma and beta emitters in geological waters in Slovenia", "Dating of the geological waters from deep aquifers" and "Validation of the method for rapid determination of the Ra-226 and Ra-228". The researchers were also involved in the other research fields related to ionising radiation and



by the micro-PIXE at the JSI tandem accelerator using a proton beam with 2 MeV energy and a 1.2 x 1.2  $\mu m^2$  cross-section. Upper row: elemental distributions of K and Zn across the whole grain (2400 x 2400 µm<sup>2</sup>). Below: elemental distributions of Mg and Fe in the aleurone layer  $(130 \times 130 \mu m^2)$  over the area indicated in the elemental map of K (upper left) with a white square. Measurements were done in collaboration with Katarina Vogel-Mikuš from the Biotechnical Faculty, the University of Ljubljana, and Sudhir Singh from the National Agri-Food Biotechnology Institute New Delhi Mohali, Punjab, India.

nuclear physics. From the bibliography, it follows that the achievements of the researchers in 2011 were solid. In addition to the basic science activities, the Group was active in conducting the radiological monitoring of the living environment in Slovenia, radiological monitoring of the fodder in Slovenia, regular off-site radiological monitoring around the Krško NPP, independent verification of the regular radiological monitoring around the Krško NPP, central radioactive waste repository radiological monitoring, monitoring of the radioactivity in drinking water, intercomparisons, proficiency tests, material characterizations, calibrations of the radiation gauges and the TLD measurements of the personal and environmental doses.

In the Laboratory for Dosimetric Standards the scope of the accreditation was expanded to the calibration measurements for the RQR and RQA photon beam qualities. The Group thrived in winning new projects from the EU funding – the EMRP projects: Metrology of Ionising Radiation in Metallurgical Industry (MetroMetal) and Metrology for Radioactive Waste Management (MetroRWM). In collaboration with the SCK-CEN, Belgium, the "Training course on environmental risk assessment, the ERICA tool and atmospheric dispersion modelling" was organized.

The members of the Infrastructure Group also took part in regular drills and special tasks with the radiological mobile unit. The members of the mobile unit participated in: international dose rate intercomparison measurements in Ronneburg, Germany, international intercomparison exercise of the in-situ gamma-ray spectrometry, dose rate and contamination measurements "ISI Gamma 2011" in Davos, Switzerland, special presentation day "Days of Protection and Rescue" in Koper and radiological emergency exercise "INEX-4" in Slovenske Konjice.

#### Some outstanding publications in 2011

- P. Lablanquie, F. Penent, J. Palaudoux, L. Andrić, P. Selles, S. Carniato, K. Bučar, M. Žitnik, M. Huttula, J. H. D. Eland, E. Shigemasa, K. Soejima, Y. Hikosaka, I. H. Suzuki, M. Nakano, in K. Ito, "Properties of Hollow Molecules Probed by Single-Photon Double Ionization". *Phys. Rev. Lett.*, **106**, 063003 (2011).
- P. Lablanquie, T. P. Grozdanov, M. Žitnik, S. Carniato, P. Selles, L. Andrić, J. Palaudoux, F. Penent, H. Iwayama, E. Shigemasa, Y. Hikosaka, K. Soejima, M. Nakano, I. H. Suzuki, in K. Ito, "Evidence of Single-Photon Two-Site Core Double Ionization of C<sub>2</sub>H<sub>2</sub> Molecules". *Phys. Rev. Lett.*, **107**, 193004 (2011).
- J. Hoszowska, J.-Cl. Dousse, J. Szlachetko, Y. Kayser, W. Cao, P. Jagodzinski, M. Kavčič, S.H. Nowak, "First Observation of Two-Electron One-Photon Transitions in Single-Photon K-Shell Double Ionization". *Phys. Rev. Lett.* 107, 053001 (2011).
- E. Krishnakumar, S. Denifl, I. Čadež, S. Markelj, N. Mason, "Dissociative electron attachment cross sections for H<sub>2</sub> and D<sub>2</sub>". *Phys. Rev. Lett.* **106**, 243201 (2011).
- 5. H. Merkel et al. (A1 Collaboration), Phys. Rev. Lett. 106 (2011) 251802.

#### Awards and appointments

- 1. Prof. Dr. Alojzij Franc Kodre: Gold Medal of the University of Ljubljana for scientific, educational and organizational work at the Faculty of Physics
- 2. Dr. Matjaž Vencelj: Fruitful collaboration and business partnership award, Ljubljana, Fotona d.d.

#### Organization of conferences, congress and meetings

1. Training course on environmental risk assessment: ERICA tool and atmospheric dispersion modelling, Ljubljana, 24–26 October 2011

# INTERNATIONAL PROJECTS

- Support of Public and Industrial Research Using Ion Beam Technology SPIRIT
   PP, 227012, FP7-INFRASTRUCTURES-2008-1
   FC, Bref, Wolfbard Möller, Forschungszentrum Disorden Research of V. Disorden Research and Statistical Sciences (Neurophysics)
  - EC; Prof. Wolfhard Möller, Forschungszentrum Dresden-Rossendorf e.V., Dresden, Germany Asst. Prof. Primož Pelicon

 Application of Ion Beam Analytical Method to the Studies of Plasma Wall Interaction in Tokamaks - 1.4.3.-FU; Post Mortem Analysis of Fuel Retention with Micro-NRA for Gas Balance and ITER Prediction; WP11-PWI-01-01-01/PS EURATOM - MHEST

7. FP - EURATOM, Slovenian Fusion Association – SFA

Annex 2, 3211-08-000102, FU07-CT-2007-00065

EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Primož Pelicon

- Hydrogen/Deuterium Molecule Wall Interaction; Processes with Neutral Hydrogen Atoms and Molecules - 1.4.1.-FU EURATOM - MHEST
   F.P - EURATOM, Slovenian Fusion Association - SFA 3211-08-000102, FU07-CT-2007-00065
   EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Dr. Iztok Čadež
   Ionising Radiation Metrology for the Metallurgical Industry MetroMetal EMRP, IND04
   EURAMET e.V., Braunschweig, Germany; Centro de investigaciones energeticas, medioambientales y technologicas (CIEMAT), Madrid, Spain Branko Vodenik, M. Sc.
- 5. Metrology for Radioactive Waste Management

MetroRWM

EMRP

EURAMET e.V., Braunschweig, Germany; Cesky Metrologicky Institut Brno, Brno, Czech Republic

Branko Vodenik, M. Sc.

 Complementing the X-ray Spectrometry Activities with Micro-Beam Facility for Different Applications; Micro-analytical Techniques Based on Nuclear Spectrometry for Environmental Monitoring and Material Studies 15955/R0

IAEA, Vienna, Austria Dr. Peter Kump

- 7. IAEA Fellowship for Ms Valentina Veselinova Lyubomirova BUL/11011
  - IAEA, Vienna, Austria
- Prof. Žiga Šmit
- Archaeometric Investigations of Archaelogical Artifacts from Albania and Slovenia BI-AL/10-11-003 Prof. Aferdita Vevecka-Priftaj, Polytechnic University of Tirana, Tirana, Albania
- Prof. Žiga Šmit
- Convention de mise a disposition Contract between CNRS and JSI dtd. 27.5.2004 Letter N/REF: NS/MD/CONV/04FRE2681 [S/2004 dtd. 8.9.2004
- Dr. Paul Indelicato, Laboratoire Kastler-Brossel (LKB UMR 8552), Ecole Normale Superieure, Paris, France Dr. Iztok Čadež
- Measurement of 3H Activity in Natural Waters with Electrolytic Enrichment BI-HR/10-11-009
  - Dr. Jadranka Barešić, Ruđer Bošković Institute, Zagreb, Croatia
- Dr. Jasmina Kožar Logar 11. Dynamics at Nanoscale
  - Dinamiche su scala nanometrica
  - BI-IT/11-13-011

Dr. Lorenzo Avaldi, Istituto di Metodologie Inorganiche e dei Plasmi (IMIP), Monterotondo Scalo (Rome), Italy Asst. Prof. Matjaž Žitnik

 Target Manuipulator PO 2011-0247

Dr. Javier Flores Maldonado, Instituto Nacional de Investigaciones Nucleares (ININ), Carretera México-Toluca S/N, Ocoyoacac, Estado de México, Mexico Asst. Prof. Primož Pelicon

- Development and Support of Java Applications for Use in DESY Accelerator Control Attachment #8, 9, 10
- Dr. M. Clausen, DESY (Deutsches Elektronen Synchrotron), Hamburg, Germany Asst. Prof. Matej Lipoglavšek, Dr. Mark Pleško
- Hadron Structure in Chiral Quark Models vs. Lattice QCD BI-PL/10-11-018

Prof. Wojciech Broniowaski, H. Niewodniczanski, Institute of Nuclear Physics, Polish Academy of Science, Krakow, Poland Prof. Simon Širca, Prof. Bojan Golli

- The Chemical Cosmos: Understanding Chemistry in Astronomical Environments COST CM0805
- EC; COST Office, Brussels, Belgium Dr. Iztok Čadež
- 16. Studies of Short-Range Correlations
- BI-US/11-12-033

Dr. Shalev Gilad, Massachusetts Institute of Technology (MIT), Laboratory for Nuclear Science, Cambridge, MA, USA Prof. Simon Širca

# R &D GRANTS AND CONTRACTS

1. Development of Cherenkov radiation detector Prof. Simon Širca

# MENTORING

#### Ph. D. Thesis

1. David Jezeršek, Ion beam analysis of geometrically structured samples (mentor Žiga Šmit).

- Investigation of plant ion homeostasis using elemental imaging by laser ablationinductively coupled plasma mass spectrometry (basic research project) Asst. Prof. Primož. Pelicon
- 3. Research of the ionome of selected mycorrhizal plants
- Asst. Prof. Primož Pelicon 4. Sustainable land use in relation to soil and crop quality
- Prof. Nives Ogrinc5. Archaeologies of hunter-gatherers, farmers and metallurgists: Cultures, populations, palaeoeconomies and climate
- Prof. Nives Ogrinc 6. Mapping in tokamak walls and inside biological cells
- Asst. Prof. Primož Pelicon 7. Natural and man-made gamma- and beta rav-
- Natural and man-made gamma- and beta ray- emiters in underground waters in Slovenia Dr. Matjaž Aleš Korun
- Natural hydrochemical background and dynamics of groundwater in Slovenia Dr. Jasmina Kožar Logar
- Groundwater age determination in deep aquifers of Slovenia Dr. Jasmina Kožar Logar
- Complex hyperspectral system for automatic analysis and control of pharmaceutical pellet coating processes
   Dr. Peter Kump
- The use of specific methods for determination and prevention of adulteration of milk and dairy products Dr. Marijan Nečemer

## RESEARCH PROGRAMS

- Mobile archaeological heritage: archaeological and archaeometric investigations Prof. Žiga Šmit
- Subject as representation: taste, respect, strenght (Investigation of Slovenian material culture)
   Dr. Mariian Nečemer
- Structure of hadronic systems
- Prof. Simon Širca
- Studies of atoms, molecules and structures with photons and particles Asst. Prof. Matjaž Žitnik

# NEW CONTRACTS

- 1. Off-site radiological monitoring of NPP Krško 2011-2013 Nuclear Power Plant Krško Asst. Prof. Matej Lipoglavšek
- Monitoring of radioactivity in the living environment in Slovenia 2011-2012 Ministry of the Environment and Spatial Planning
- Dr. Benjamin Zorko 3. Ecology laboratory with mobile unit Ministry of Defence
- Asst. Prof. Matej Lipoglavšek
- Monitoring of central LILW storage facility at Brinje 2011 ARAO Agency for Radwaste Management Dr. Marijan Nečemer
- Annex No. 4: Professional activities and fulfilment of obligations of the holder of the national measurement standard in the field of ionizing radiation 2011 Ministry of Higher Education, Science and Technology Denis Glavič Cindro, M. Sc.
- Calibration of dosemeters for environmental dose rate measurements Ministry of the Environment and Spatial Planning Matjaž Mihelič, M. Sc.

# VISITORS FROM ABROAD

- 1. Dr. Davor Peruška and Dr. Suzana Petrovič, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 28 March to1 April 2011
- Prof. Dr. Aferdita Vevecka Priftaj, Polytechnic University, and Assoc. Prof. Frederik Stamati, Albanian Archaeological Institute and Museum, Tirana, Albania, 26 June to 1 July 2011
- Dr. David Dominguez-Villar, University of Alcalá de Henares, Alcalá de Henares, Spain, 18–25 June 2011
- 4. Ebrahim Gholami Hatam, Vaan de Graaf Generator Laboratory, Teheran, Iran, 22 June to 25 December 2011

- Wojciech Lubarski, Poznan University of Technology, Poznan, Poland, 4 July to 26 5. August 2011
- 6 Dr. Olga Ogorodnikova, IPP, Garching, Germany, 8-19 August 2011
- Dr. Paula Chavez and Ana Taborda, Instituto Tecnológico e Nuclear, Sacavém, Portugal, 19-24 September 2011

## STAFF

#### Researchers

- Prof. Iztok Arčon\*
- 2. Dr. Klemen Bučar
- Prof. Dean Cvetko\* 3.
- Dr. Iztok Čadež
- Denis Glavič Cindro, M. Sc. 5.
- 6. Dr. Darko Hanžel
- Asst. Prof. Matjaž Kavčič
- Prof. Alojzij Franc Kodre' 8
- 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. Branko Vodenik, M. Sc.
- 19. Asst. Prof. Matjaž Žitnik

#### Postdoctorial associates

- 20. Dr. Jasmina Kožar Logar
- 21 Dr Sabina Markeli
- Dr. Paula Pongrac
   Dr. Zdravko Siketić, left 01.09.11
- 24. Dr. Matjaž Venceli

#### 25. Dr. Benjamin Zorko

# BIBLIOGRAPHY

#### ORIGINAL ARTICLES

- 1. Patrick Achenbach et al. (21 authors), "Particle tracking in kaon electroproduction with cathode-charge sampling in multi-wire propotional chambers", Nucl. instrum, methods phys res., Sect. A, Accel., vol. 641, pp. 105-113, 2011.
- 2. Patrick Achenbach et al. (27 authors), "A large-scale FPGA-based trigger and dead-time free DAQ system for the kaos spectrometer at
- MAMI", *IEEE trans. nucl. sci.*, vol. 58, no. 4, pp. 1677-1684, 2011. 3. P. Bourgeois *et al.* (37 authors), "Measurements of the generalized electric and magnetic polarizabilities of the proton at low  $Q^2$  using the virtual Compton scattering reaction", Phys. rev. C. Nucl. phys., vol. 84, pp. 035206-1-035206-8, 2011.
- 4. W. Cao, J.-Cl. Dousse, J. Hoszowska, Matjaž Kavčič, Y. Kayser, J. L. Schenker, Matjaž Žitnik, "Double L3M ionization of Pd induced by impact with medium-energy electrons", Phys. rev., A, vol. 83, no.2, pp. 022708-1-022708-11, 2011.
- 5. W. Cao et al. (12 authors), "High-resolution KMM radiative Auger x-ray emission spectra of calcium induced by synchrotron radiation", Phys. rev., A, vol. 83, no. 4, pp. 042513-1-042513-9, 2011.
- 6. Albano Cossaro, Michele Puppin, Dean Cvetko, Gregor Kladnik, Alberto Verdini, Marcello Coreno, Monica de Simone, Luca Floreano, Alberto Morgante, "Tailoring SAM-on-SAM formation", J. phys. chem. lett., vol. 2, no. 24, pp. 3124-3129.
- 7. Iztok Čadež, Milan Čerček, Zvone Grabnar, Sabina Markelj, Primož Pelicon, Zdravko Rupnik, Vida Žigman, "Processes with neutral hydrogen atoms and molecules", Annual report ..., pp. 17-22, 2011.
- 8. Iztok Čadež, Sabina Markelj, Aleksandar R. Milosavljević, "Influence of hydrocarbons on vibrational excitation of H[sub]2 molecules", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, issue 4, pp. 1267-1271, 2011.

- Dr. Zsófia Kertész and Eniko Furu. Institute of Nuclear Research of the Hungarian 8. Academy of Sciences (ATOMKI), Debrecen, Hungary, 25 September to 1 October 2011
- 9 Dr. Ines Krajcar Bronić, Ruđer Bošković Institute, Zagreb, Croatia, 6-12 November 2011
- 10. Dr. Jadranka Barešić, Ruđer Bošković Institute, Zagreb, Croatia, 10-12 November 2011
- 11. Dr. Peter O 'Keeffe, CNR-IMIP, Rome, Italy, 15-19 November 2011

#### Postgraduates

- 26. Jure Beričič, B. Sc. 27. Rok Bohinc, B. Sc. 28. Luka Debenjak\*\* 29. Helena Fajfar\*\* 30. Jelena Gajević, B. Sc. 31. Nataša Grlj, B. Sc. 32. Luka Jeromel, B. Sc. 33. Dr. David Jezeršek, left 01.11.11 34. Katarina Kovačič, B. Sc. 35. Miha Mihovilovič, B. Sc 36. Mojca Miklavec, B. Sc. **Technical officers** 37. Boštjan Črnič, B. Sc 38. Matjaž Mihelič, M. Sc. 39. Primož Vavpetič, B. Sc. Technical and administrative staff 40. Drago Brodnik 41. Moica Gantar 42. Sandi Gobec 43. Zvonimir Grabnar
- 44. Mirko Ribič, B. Sc.

#### Note:

- \* part-time JSI member \*\* postgraduate financed by industry
- 9. Robert Dominko, Candela Vidal-Abarca Garrido, Marjan Bele, Mirjana Küzma, Iztok Arčon, Miran Gaberšček, "Electrochemical characteristics of Li2 - xVTiO4 rock salt phase in Li-ion batteries", In: IMLB 2010, J. Power Sources, vol. 196, no. 16, pp. 6856-6862, 2011.
- 10. Mihael Drofenik, Irena Ban, Darko Makovec, Andrej Žnidaršič, Zvonko Jagličić, Darko Hanžel, Darja Lisjak, "The hydrothermal synthesis of super-paramagnetic barium hexaferrite particles: review", Mater. chem. phys., vol. 127, iss. 3, pp. 415-419, 2011.
- 11. Johannes Teun van Elteren, Zdenka Šlejkovec, Iztok Arčon, Michael Philip Beeston, Andrej Pohar, "Multiple kinetic Langmuir modeling to predict the environmental behaviour of As(V) in soils", J. environ. monit. (Print), vol. 13, no. 6, pp. 1625-1633, 2011.
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#### TEXTBOOKS AND LECTURE NOTES

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#### THESES

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#### PATENT APPLICATION

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# DEPARTMENT OF THIN FILMS AND SURFACES

F-3

The main field of research in 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.

As in previous years, the main emphasis of the R&D work has remained in the field of hard protective coatings. The work has mainly been application-oriented, both in the implementation of coatings into industrial production and in advanced analysis after using these coatings.

A lot of work has been dedicated to nanocomposite and nanolayer coatings based on (Ti,Al,Si)N. The nanolayer structure is achieved by the simultaneous deposition from two different targets. In practice this is done by rotation of the samples (i.e., substrates) in the deposition chamber. At a given moment the material from the target facing Head: the sample enables the growth of a particular layer. The formation of a nanocomposite coating is possible only if *Dr. Peter Panjan* the kinetic conditions of spontaneous phase separation are met. In our case these are the TiN or TiAlN grains of

about 10 nm size in a matrix of amorphous Si<sub>2</sub>N<sub>4</sub>. We analysed the influence of the deposition parameters (target power, gas flow) on the microstructure and on the mechanical properties (hardness, adhesion). Nanolayer and nanocomposite coatings were analysed by transmission electron microscopy, while the chemical state of the individual elements was evaluated using X-ray photoelectron spectra (XPS).

The lifetimes of cemented-carbide cutting inserts coated with the (Ti,Al,Si)N coating were evaluated in the Faculty for Mechanical Engineering at the University of Ljubljana. During the milling of a workpiece with a hardness of 57 HRC and without cooling liquids we changed both the cutting speed and the feed. We measured the cutting force and the workpiece roughness, and analyzed the wear. The optimal machining parameters were determined using the Taguchi method. Identical tests were made by the cutting inserts, protected by the nanolayer AlTiN/TiN-based coating ("blue coating").

The preparation and characterization of nanostructured coatings is the topic of two PhD theses by two foreign young researchers: Halil Çalışkan (Bartın University, Turkey) and Aleksandar Miletić (University of Novi Sad, Serbia). Both performed most of their experimental work in our lab.

In some niche applications (hard and dry machining) the (Ti,Al,Si)N coating was successfully implemented into industrial production.

For several years we have studied the growth defects that arise during the deposition of hard coatings and have a detrimental influence on the corrosion resistance and the tribological properties (increased wear, sticking of workpiece material). Last year we systematically analysed the role of this type of defects in crevice corrosion. For this research, we used 3D profilometry and SEM microscopy in combination with a focused ion beam (FIB). Using the appropriate software we were able to conduct a 3D reconstruction of individual defects in order to better understand their formation mechanism. This work was done in collaboration with the Faculty of Mechanical Engineering from Maribor, and this work is the topic for one of our young researcher's PhD thesis.

A novelty in our research work is the so-called triangular targets. The idea is to substitute a monolithic target with a pair of triangular targets with different compositions, which enables the deposition of a composition gradient along the chamber's vertical axis. In this way a set of samples with





Figure 1: Cross-section HRTEM image of the nanocomposite coating TiSiN, which is composed of TiN nanograins and Si  $N_{a}$  amorphous phase (author: Asst. Prof. Goran Dražić)

We developed an AICuFeB quasicrystalline coating. In combination with a TiAIN interlayer it enables the protection of tools for the milling of carbon steel. This achievement overlaps with last year's Nobel Prize for the discovery of quasicrystals.



Figure 2: Cutting and forming tools, coated by the AICuFeB quasicrystalline coating

different compositions is deposited in a single process. We first applied this principle for the pair Cr/Al, which was added to the existing classic TiSi targets. Thus we were able to deposit coatings with a range of compositions from TiCrSiN to TiAlSiN. The last such test was the deposition of the gradient Cr<sub>2</sub>V<sub>1</sub> N.

Nanolayer and nanocomposite coatings are also a topic of the Nano Tool project (ERA-SME). Within this project we are developing the coatings for the protection of cutting and forming tools under specific wear conditions.

We increased our efforts in the tribological characterization of the "black coating " (TiAlN/a-CN). We measured the wear resistance and friction coefficient in dependence of the deposition parameters and measuring conditions.

Last year the AppliCMA project came to a conclusion (7. FP, Development of wear resistant coatings based on complex metallic alloys for functional applications). Within this project we developed the quasicrystalline coating AlCuFeB, which was successfully deposited on cutting tools and plastic injection tools. Sufficient adhesion was achieved by the deposition of the TiAlN interlayer. The tools were tested at different project partners and we found that the results for the milling of carbon steel are comparable to those obtained with commercial coatings.

We are engaged in several domestic projects, co-financed by companies. For the company Impol we are developing colour coatings on wrought aluminium workpieces, and protective coatings for aluminium extrusion tools. In collaboration with the National Institute of Chemistry and the company Cetis (Celje) we are developing a process for hologram formation in security printing. The protection of Sm-Co magnets for high-temperature applications is the topic of a joint project with the company Magneti (Ljubljana).

We also started the development of nanostructured multifunctional coatings for improvement of the surface properties of metals and alloys, applied as implants in the human body. Coatings based on TiN, (Ti,Si)N and TaN with added silver or copper show an antibacterial behaviour, in addition to good corrosion and

tribological properties. In this applied project we are collaborating with the company Gazela (Krško). In the broad area of bioapplications we are studying the corrosion and tribological properties of diamond-like carbon coatings deposited on stainless-steel substrates. We have continued our work on Al-W coatings for the corrosion protection



Figure 3: Cross-section TEM image of the "black coating" (TiAlN/a-CN). This coating has a high wear resistance and a low friction coefficient. The tools which we protected by the black coating have been successfully implemented in industrial production of several companies (Unior, Silgan, Krka).

of aluminium alloys. The results showed that the corrosion resistance of aluminium alloys increases by two to three orders of magnitude if protected by an Al-W coating with the proper composition and microstructure.

There are many more informal cooperations with different companies, even after a project has expired. This work is usually carried out as an investigation, where we solve specific advanced technological problems.

At the level of basic sciences we collaborate with several foreign partners. We have an on-going bilateral project with the Institute of Physics of the Czech Academy of Sciences from Prague; the main scope of the project is the deposition and characterization of colour coatings. Though we have no current project with the Austrian Joanneum Research any more, the collaboration goes on, especially in corrosion studies of diamond-like carbon coatings. A similar informal collaboration has continued with the Vinča Institute from Belgrade, performing radiation damage crater analysis after a pulsed laser treatment. 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.

We are also collaborating with the École Polytechnique from Montreal were our coworker, Dr Matjaž Panjan, is currently on a one-year postdoctoral stay. His research work is connected to the various advanced hard coatings that are deposited by high-power pulsed magnetron sputtering. This is also a topic of an on-going national project "Development of a new generation of hard coatings by pulsed sputtering ".

#### Some outstanding publications in the past year

 Corrosion properties of DLC-coated stainless steel in hanks solution for biomedical applications, Darja Kek Merl, Peter Panjan, Miha Čekada, Markus Kahn, Wolfgang Waldhauser, *ECS Transactions* 35 (2011) 7, 67–73

- 2. Tribological properties of diamond-like carbon coatings prepared by anode layer source and magnetron sputtering, Srečko Paskvale, Markus Kahn, Miha Čekada, Peter Panjan, Wolfgang Waldhauser, Bojan Podgornik, Surf. coat. technol. 205 (2011) 2, S99-S102
- 3. Hydrogen permeation through TiAlN-coated Eurofer '97 steel, Paul J. McGuiness, Miha Čekada, Vincenc Nemanič, Bojan Zajec, Aleksander Rečnik, Surf. coat. technol. 205 (2011) 8/9, 2709-2713



Figure 4: Surface morphology of the TiVN coating after oxidation at 750 °C

# INTERNATIONAL PROJECTS

1. Development of Wear Resistant Coatings based on Complex Metallic Alloys for Functional Applications

appliCMA 7. FP, 214407

EC; Andreas Merstallinger, Aerospace & Advanced Composites GmbH, Wiener Neustadt, Austria

Asst. Prof. Miha Čekada, Prof. Janez Dolinšek, Asst. Prof. Kristoffer Krnel, Asst. Prof. Srečo D. Škapin

2. Plasma Deposition of H:C-metal Coatings - 1.4.5.-FU EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association - SFA

Annex 3, 3211-08-000102, FU07-CT-2007-00065

EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Dr. Peter Panian

Hydrogen Impermeable Nano-material Coatings for Steels 3. Hy-Nano-IM

MNT ERA NET Asst. Prof. Miha Čekada, Asst. Prof. Paul McGuiness, Dr. Vincenc Nemanič

- 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
  - NANO-TOOL
  - ERASME

5

EMO-Orodjarna d.o.o., Celje, Slovenia

Dr. Peter Panjan

Deposition and Characterization of Nanostructured hard Coatings with Tailored Optical Properties

BI-CZ/11-12-007

Dr. Michal Novotny, Institute of Physics Academy of Sciences of the Czech Republic, v.v.i., Prague, Czech Republic Asst. Prof. Miha Čekada



Figure 5: Cross-section SEM image of the bilayer coating TiAlN/Al\_O\_for the protection of cutting tools, which are exposed to extreme temperatures at the cutting edge

# **R &D GRANTS AND CONTRACTS**

- Organic-inorganic thin film structures for electronic components 1. Asst. Prof. Janez Kovač
- Development of electronical measuring paltform POWERQ4 2. Dr. Peter Panjan
- A study of plasma parameters for conditioning of the inner surfaces of a fusion reactor 3. Prof. Miran Mozetič
- 4. Development of new generation of hard coatings with pulsed sputter deposition Dr. Peter Panjan
- 5. Materials and structures for optically variable security devices
- Dr. Peter Panjan 6. Protected Permanent Magnets for Advanced High-Temperature Applications Asst. Prof. Paul John Mcguiness
- Multifunctional Nanostructured Films for Artificial Implants Corrosion and Tribocorrosion Processes
- Dr. Darinka Kek Merl Research and development of rapid production and repair in modern 3D cutting tools with advanced laser technologies
- Dr. Peter Panjan Colour, absorption and protective nanolayer coatings for aluminium alloy 9. Dr. Peter Panjan
- 10. Functionalization of biomedical samples by thermodynamic non-equilibrium gaseous plasma . Prof. Miran Mozetič
- 11. Toward ecologically benign alternative for cleaning of delicate biomedical instruments Asst. Prof. Alenka Vesel

# RESEARCH PROGRAM

Thin film structures and plasma surface engineering 1 Prof Miran Mozetič

# VISITORS FROM ABROAD

- Halil Çalişkan, MSc, Bartın University, Faculty of Engineering, 74100 Bartın, Turkey, 19. 1. - 30. 9. 2011
- 2. Dr. Bojan Radak, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 14.-15. 2. 2011
- Vladimír Jech, Dana Benešová, Czech Technical University, Prague, Czech Republic, 18.–30. 4. 2011
- Aleksandar Miletić, Pal Terek, University of Novi Sad, Novi Sad, Serbia, 1. 7. 31. 8. 2011
   Dr. Jiří Bulíř, Institute of Physics of the Academy of Sciences of the Czech Republic,
- Prague, Czech Republic, 12.–17. 7. 2011
  Dr. Michal Novotný, Dr. Petr Pokorný, Institute of Physics of the Academy of Sciences of the Czech Republic, Prague, Czech Republic, 8.–12. 8. 2011
- STAFF Researchers

#### Asst. Prof. Miha Čekada

Dr. Darinka Kek Merl

#### 3. Dr. Peter Panjan, Head

#### Postdoctorial associates

#### 4. Dr. Matjaž Panjan

#### Postgraduates

Peter Gselman, B. Sc.
 Vladan Mladenović, M. Sc.\*\*

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- 7. Paul J. McGuiness, Miha Čekada, Vincenc Nemanič, Bojan Zajec, Aleksander Rečnik, "Hydrogen permeation through TiAlN-coated Eurofer '97 steel", *Surf. coat. technol.*, vol. 205, no. 8/9, pp. 2709-2713, 2011.
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- 8. Aleksandar Miletić, Pal Terek, University of Novi Sad, Novi Sad, Serbia, 3.-14. 10. 2011
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- 10. Dr. Christoph Schiffers, CemeCon A.G., Würselen, Germany, 24. 11. 2011
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7. Srečko Paskvale, B. Sc.

- Technical and administrative staff
- 8. Jožko Fišer
- 9. Damjan Matelič 10. Andrej Mohar
- 11. Tomaž Sirnik

#### Note:

\*\* postgraduate financed by industry

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#### **Invited** Paper

 Peter Panjan, Srečko Paskvale, Peter Gselman, Franc Zupanič, Tonica Bončina, Miha Čekada, Matjaž Panjan, Darja Kek-Merl, B. Fišinger, "Tribological properties of a-CN<sub>x</sub> coating", In: *Conference proceedings*, 8th International Conference on Industrial Tools and Material Processing Technologies [also] ICIT & MPT, Ljubljana, Slovenia, October 2nd - 5th 2011, Janez Marko Slabe, ed., Celje, TECOS, Slovenian Tool and Die Development Centre, 2011, pp. 337-342.

#### **Regular** papers

- 1. Halil Çalişkan, Davorin Kramar, Peter Panjan, C. Kurbanoglu, Miha Čekada, Janez Kopač, "Evaluation of wear behavior of TiAlSiN/TiSiN/TiAlN multilayer nanocomposite coating in face milling of hardened steel", In: *Conference proceedings*, 8th International Conference on Industrial Tools and Material Processing Technologies [also] ICIT & MPT, Ljubljana, Slovenia, October 2nd - 5th 2011, Janez Marko Slabe, ed., Celje, TECOS, Slovenian Tool and Die Development Centre, 2011, pp. 343-348.
- 2. Halil Çalişkan, Davorin Kramar, Peter Panjan, C. Kurbanoglu, Janez Kopač, "Influence of hard coatings and cutting parameters on cutting performance and surface quality in hardened steel milling", In: MIT & SLIM 2011: proceedings of the 11th International Conference on Management of Innovative Technologies & 2nd International Conference on Sustainable Life in Manufacturing, Fiesa, Slovenia, September 25th 27th, 2011, Mihael Junkar, ed., Janez Kopač, ed., Paul R. Levy, ed., Oguz Colak, ed., Ljubljana, TAVO, Slovene Society for Abrasive Water Jet Technology, 2011, pp. 109-116.
- 3. Halil Çalişkan, Davorin Kramar, Peter Panjan, C. Kurbanoglu, Janez Kopač, "Investigation of the wear behaviour of carbide cutting tools coated with AlTiN/TiN nanolayer hard coating in hard milling", In: *MIT & SLIM 2011: proceedings of the 11th International Conference on Management of Innovative Technologies & 2nd International Conference*

on Sustainable Life in Manufacturing, Fiesa, Slovenia, September 25th - 27th, 2011, Mihael Junkar, ed., Janez Kopač, ed., Paul R. Levy, ed., Oguz Colak, ed., Ljubljana, TAVO, Slovene Society for Abrasive Water Jet Technology, 2011, pp. 129-135.

- 4. Darja Kek-Merl, Peter Panjan, Miha Čekada, Markus Kahn, Wolfgang Waldhauser, "Corrosion properties of DLC-coated stainless steel in Hanks solution for biomedical applications", In: *Bioelectronics, biointerfaces, and biomedical applications*, (ECS transactions, vol. 35, no. 7, 2011), 219th ECS Meeting, May 1-May 6, 2011, Montreal, Canada, M. Madou, ed., Pennington, The Electrochemical Society, 2011, vol. 67, no. 35, pp. 67-73, 2011.
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- 6. Peter Panjan, Darja Kek-Merl, Peter Gselman, Tonica Bončina, Franc Zupanič, Matjaž Panjan, Miha Čekada, "Raziskave mehanizmov jamičaste korozije jeklenih podlag zaščitenih s TiAlN in CrN prevlekami", In: Vir znanja in izkušenj za stroko: zbornik foruma, Industrijski forum IRT, Portorož, 6. in 7. junij 2011, Tomaž Perme, ed., Darko Švetak, ed., Škofijica, Profidtp, 2011, pp. 137-142.
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# DEPARTMENT OF SURFACE ENGINEERING AND OPTOELECTRONICS F-4

The research program of the department 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 fusion-relevant materials, the thermodynamics of trapped gases and methods for sustaining an ultra-high-vacuum environment, vacuum optoelectronics, and basic research in the field of surface and thin-film characterization by electron spectroscopy techniques.

The construction of a large plasma reactor for the modification of large samples as well as for the development of plasma-based technologies for our industrial partners has been accomplished. The length of the new plasma reactor is over 2 m. The plasma is excited at moderately low pressure by a high-frequency electrical discharge. The coupling between the high-frequency generator and the plasma in large volumes is far from being trivial. Both theoretical simulations and experimental work have been performed in order to optimize the coupling. Extensive Head: theoretical investigation gave valuable results in terms of coupling efficiency and stability. The most promising Prof. Miran Mozetič configurations were realized in our workshop and experiments with suitable components of the matching network allowed for optimization in the real environment. The impedance of the secondary oscillating circuit at such large dimensions is prohibitively large, so it does not allow for application of a common induction coil due to a very high



voltage amplitude. This problem was solved using a multilayered coil which turned out to be very useful for the achievement of good plasma uniformity along the discharge vessel as well as in terms of the coupling efficiency. The original idea was protected by a patent application filed in 2011 and submitted to the Slovenian Intellectual Property Office. Such a multilayered coil allows for a rather low peak voltage and thus a substantial decrease in the stray effects caused by the capacitive component of the coupling. In comparison with standard induction coils in use worldwide the innovative approach resulted not only in a very good homogeneity of the plasma along the 2-mlong discharge vessel made from a dielectric material but also for an at least 60% better coupling efficiency at powers exceeding 5 kW.

The high-frequency discharge used for the excitation of the gaseous plasma at moderately low pressures is found either in E or H mode. The major characteristic of the E mode is the prevalence of the capacitive-coupling component between the powered electrode and the grounded one. A consequence of such a coupling is the formation of rather narrow sheaths next to the powered electrode. Free electrons gain energy from the electric field only in a sheath and are able to transfer a part of the energy to electrons



Figure 1: Gaseous plasma in the reactor with a 2-m-long discharge vessel

far from the sheath only by diffusing from the sheath into the central part of the discharge vessel. In cases of particular interest, i.e., when samples are treated by plasma in order to functionalize their surfaces or remove surface impurities or etch selectively a particular component of composite materials, such a coupling is not useful since the plasma is not homogeneous in the entire volume. Reactive particles are lost by surface reactions and could be

replaced only if the electron energy close to the samples is favorably large. In such cases it is better to keep a discharge in the H mode. The transition from E to H mode occurs at a sufficiently large density of oscillating magnetic field in the discharge chamber. The high-frequency magnetic field induces an appropriate oscillating electric field in the absence of any electrode. Free electrons oscillate in the electric field and may change their direction during collisions with molecules or atoms. If the mean free path is similar to the oscillation amplitude a resonance accumulation of electron energy

Two of our senior researchers, Prof. Miran Mozetič and Asst. Prof. Uroš Cvelbar, received the highest National Order for Innovations, **Development Achievements and Application of** Scientific Discoveries in Industrial Practice - the Puh award to the innovator.

will occur so the electrons will be able to gain enough energy for non-elastic collisions that can result in ionization or dissociation of a molecule. The H mode has therefore a unique advantage over the E mode since electrons are heated throughout a discharge vessel. Plasma in the H mode is thus rather homogeneous in the entire volume,

practically independent of the nature of the samples placed inside the vessel. The appearance of each mode depends on numerous parameters, including the gas pressure and the useful power transferred from the high-frequency generator to the charged particles in plasma. In general, a low pressure and high magnetic field density will favor the H mode of an electrical discharge.

The transitions between the E and H modes were studied in detail for a smaller plasma reactor. Both discharge and plasma parameters were measured. The transition is far from being gradual. A sudden change in the discharge volt-

#### A large plasma reactor, as a powerful source of neutral oxygen atoms in the ground state, has been developed in close collaboration with EURATOM partners.

age, current and phase shift occurs at the transition. The plasma luminosity may increase by three orders of magnitude and so does the density of the free electrons at the transition from E to H mode. A subject of particular interest is the behavior of the neutral atom density at the transition in cases when the plasma is generated in gases containing two- or multi-atom molecules. Systematic research of the neutral oxygen atom density at the transition has

been performed and a well-pronounced hysteresis was observed. The hysteresis was largest at moderately high pressures and the results of our research were published in a respected European physical journal.

Plasma created by high-frequency discharge in a dielectric vessel is thus a rich source of neutral atoms in the ground state. The atoms are suitable for modification of the surface properties of different materials. The modified surface characteristics depend on the flux of atoms onto the surface of a sample and a good control of the surface reactions needs precise adjustment of the neutral atom density in a processing chamber. The density could be adjusted by tuning discharge parameters, such as gas pressure, discharge voltage, current and the phase shift, but in applications such tuning is not always practical, especially in cases where the consumption of atoms by surface reactions changes during processing. It is much better to control and adjust the atom density in a processing chamber without changing the discharge parameters. To achieve such a configuration an innovative approach was applied. In a preferred embodiment the atom density is adjusted by mounting a movable active component into the processing chamber. The feed-back loop allows for active adjustment of the atoms' density and thus keeping the flux of atoms onto the surface of a sample independent of the surface properties or discharge parameters.



Figure 2: A hysteresis is observed at the transition of an electrode-less radiofrequency discharge between E and H modes. The hysteresis depends largely on the pressure in the discharge vessel.

This innovative approach has been also protected by a patent application.

We are partners in the European project "PlasmaNice": Atmospheric plasmas for nanoscale industrial surface processing, funded as part of the EU's 7th FP. Fifteen European partners from research and industry are involved in the project. It aims at the improvement of the recyclability of conventional fossil-fuel-based plastics for packaging and their replacement by renewable bio-based and biodegradable materials. The main objective of the PlasmaNice project is the development of technology and equipment for industrial in-line atmospheric plasma deposition of functional nanocoatings on various fibre- and polymer-based substrates for packaging. Our group carried out a precise surface characterization of plasma-deposited sol-gel coatings using XPS, AFM and SEM methods. We determined the correlation between the plasma process parameters, the degree of surface fuctionalization and the thickness of the deposited coatings. In the frame of the project we have developed a new method for the fast and in-line monitoring of the efficiency of air plasma surface activation at very high velocity, which has great potential for industrial applications.

Advanced surface analytical methods are indispensable for the characterization of the surfaces and interfaces of bulk materials, layered structures

and nanomaterials. 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 the characterization of technological samples. A new method, secondary ion mass spectroscopy (TOF-SIMS), has been introduced in our laboratories. Our research group is world recognized for the depth profiling of thin films and multilayers at a high depth resolution.

Using surface analytical methods we investigated the formation of laser-induced periodic surface structures (LIPSS) and structural changes in Ni/Ti multilayers after laser irradiation. These periodic structures have potential applications in the field of nanolitography for the patterning of gratings with periodicity in the nm range. In collaboration with the Institute for Nuclear Sciences from Vinča, Serbia, magnetron sputtering was used to deposit (Ni/Ti)  $\times$  5 multilayers on a Si substrate with the thickness of the individual layer being 18 nm. Laser irradiation was performed with a Nd:YAG laser, operating at 1064 nm wavelength and with a pulse duration of 150 ps. The samples were treated with 100 and 200 pulses, the laser pulse energy was of 55 mJ and the total fluence was about 1 J/cm<sup>2</sup>. The composition and surface morphology were monitored by Auger electron spectroscopy (AES) and by atomic

force microscopy (AFM). Unexpectedly, we found the formation of a regularly rippled surface topography with a periodicity of 780 nm and a height of the ripples of 5–15 nm. This periodicity depends on the laser wavelength, the polarization and the angle of incidence. Depth profile AES analyses revealed that laser annealing also induced

intermixing between the individual Ni and Ti layers with indications of the possible formation of Ni–Ti intermetallic compounds. An interesting outcome is the surface segregation of Ti, although the original topmost layer prior to laser irradiation was Ni.

An innovative permeation technique enabling the resolution of extremely low hydrogen fluxes with subsequent quantitative analysis has been

invented. The technique has been applied for studying the interaction of hydrogen with fusion-relevant materials. Special attention was devoted to the suppression of a hydrogen background from the heated sample holder. Permeation measurements through various duplex membranes were realized. The fusion-relevant materials were deposited as thin films on Eurofer (a special stainless-steel material suitable as a construction material for future

fusion reactors) substrates. The activities were performed within Euratom and EFDA projects. In cooperation with dr. W. Waldhauser at Joanneum Research Centre in Leoben (Austria) we found that silicon oxy-nitride and silicon nitride films could be prepared in a form with a very high permeation reduction factor (PRF). It was shown that 0.5-micrometer-thick SiN films have the highest PRF ever reported for such thin materials.

Pure beryllium, tungsten and mixed beryllium/tungsten films deposited onto Eurofer were investigated in this context, too. Both pure metals are intended to be applied as first-wall materials in future large fusion reactors, and thin films of mixed deposits are supposed to accumulate on the cooled walls of reactors during operation with a hot hydrogen plasma. Several beryllium and Be/W films were deposited in dr. Cristian Lungu's lab at "National Institute for Laser, Plasma and Radiation Physics" (NILPRP), Bucharest, Romania, using their thermionic vacuum arc method. Relatively reproducible results have been obtained. So far, no data on the permeation of such films have been reported. The unexpected kinetics could be well explained by our improved model and respecting the fact that data on bulk Be are rather old and inaccurate.

An investigation of the permeability of tungsten films deposited onto the Eurofer alloy by pulsed laser deposition (PLD) was realized for the first time. Tungsten films (1 and 10  $\mu m$  thick) were provided by dr. Matteo Passoni at Politecnico di Milano, Italy. Their main feature was a nanocrystalline

structure, which resulted in an over two orders of magnitude lower permeability compared to the values obtained for W films deposited by the combined magnetron sputtering and ion implantation (CMSII). Moreover, the hydrogen content in W films deposited by the PLD method was as high as  $\sim 0.1$  H/W. Such high ratios have been reported only for hydrogen storage materials. These unexpected results are in agreement with theoretical models reported recently.

Our studies on thermionic energy conversion within a bilateral project with our partner at Arizona State University revealed that besides the structure of a nanostructured diamond film hydrogen plays the key role in achieving an extremely low work function. Hydrogen could be incorporated in the topmost layer just after the synthesis and also at any later time to recover the loss caused by its slow evaporation at elevated temperatures. **Our report on hysteresis i** 

Our improved set-up for quantitative gas analysis was successfully applied also in an investigation of the breakdown-voltage drift with time in gas surge arresters. Consequently, with the proper gas mixture and thermal treatment, an extremely stable breakdown voltage was achieved. Optimized coupling between the RF generator and the gaseous plasma allows for a dissociation fraction of the oxygen molecules exceeding 99% at room gas kinetic temperature.



Figure 3: Surface topography and depth distribution of elements in the multilayered (Ni/Ti)x5/Si nanocomposites upon laser irradiation with 100 and 200 pulses. Unexpectedly, the laser induced periodical surface structures (LIPSS) were formed with a periodicity of 780 nm.

Our report on hysteresis in neutral oxygen atom density at the discharge transition from E to H mode was published in a respected European physical journal: Europhysics letters.

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.

The new open-pore rigid organic foams, which are stable at temperatures up to 200°C, were synthesized at the Melamin Company from Kočevje, Slovenia. Using our extremely sensitive techniques it was revealed that they also have an extremely low outgassing rate. Their low thermal conductivity, equal to 6 mW/(mK), and low cost in continuous production, make them extremely attractive as the core material in vacuum insulating panels (VIP). Novel VIP solutions are the most promising approaches towards energy-efficient devices and buildings.

#### Some outstanding publications in the past year

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- Zajec, Bojan, Nemanič, Vincenc, Žumer, Marko, Bryan, Eugene N., Nemanich, Robert J. Ring-shaped field emission patterns from carbon nanotube films. Carbon (N. Y.). [Print ed.], 2011, vol. 49, issue 10, str. 3332-3339, doi: 10.1016/j.carbon.2011.04.020.

#### Patent granted

 Method for synthesis of magnetic liposomes in electric field Kristina Eleršič, Miran Mozetič, Alenka Vesel, Janez Pavlič, Aleš Iglič, Andrej Žnidaršič, Aljoša Košak SI23095 (A), Urad RS za intelektualno lastnino, 31.1.2011.

#### Awards and Appointments

1. Two senior researchers received the highest Slovenian prize for innovations and knowledge transfer to industrial production – the Puh award.

#### Organization of Conferences, Congresses and Meetings

- 2nd International Workshop on Plasma Nano-Interfaces and Plasma Diagnostics, Cerklje, Slovenia, 1<sup>st</sup> 3<sup>rd</sup> April 2011
- 2. 18th International Scientific Meeting on Vacuum Science and Techniques, Bohinj, Slovenia, 2<sup>nd</sup> 3<sup>rd</sup> June 2011
- 3. 112 IUVSTA executive council meeting, Strunjan, Slovenia, 9th 11th September 2011
- 4rd International Conference on Advanced Plasma Technologies (ICAPT-IV), Strunjan, Slovenia, 11<sup>th</sup> –13<sup>th</sup> September 2011

# INTERNATIONAL PROJECTS

1. Atmospheric Plasmas for Nanoscale Industrial Surface Processing PlasmaNice

7. FP

EC; Dr. Johanna Lahti, Tampere University of Technology, Paper Converting and Packaging Technology, Tampere, Finland

- Asst. Prof. Janez Kovač
- Removal of Deposits by Neutral Oxygen and Nitrogen Atoms 1.4.2. FU WP10-PWI-02-02/MHEST/PS; Detailed Characterization of Reaction Products from Removal of A-C:H with Mixed H2/N2 Plasmas
   WP111 PWI-02-04 (1.4 Application of Neutral Atoms for Evel Removal in Cons.
  - WP11-PWI-02-04-01; Application of Neutral Atoms for Fuel Removal in Gaps EURATOM – MHEST
  - 7. FP EURATOM, Slovenian Fusion Association SFA
  - Annex 3, 3211-08-000102, FU07-CT-2007-00065
  - EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Prof. Miran Mozetič
- Deuterium Interation Kinetics Metals Relevant to Iter or Demo 1.4.4. FU WP11-PWI-01-02-01/PS; Hydrogen Permeability of W/BE Films EURATOM – MHEST
- 7. FP EURATOM, Slovenian Fusion Association SFA

Annex 3, 3211-08-000102, FU07-CT-2007-00065

- EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Dr. Vincenc Nemanič
- Plasma Sterilization and Decontamination of Water NATO CLG. REF.983580

Dr. Fausto Pedrazziini, NATO - North Atlantic Treaty Organisation, Brussels, Belgium Asst. Prof. Uroš Cvelbar

- Development of Bioactive Packaging
- BIOPAĈKAGING EUREKA

Univerza v Mariboru, Inštitut za inženirske materiale in oblikovanje, Maribor, Slovenia Prof. Miran Mozetič

- 6. Hydrogen Impermeable Nano-material Coatings for Steels Hy - Nano – IM
  - MNT ERA NET
- Dr. Vincenc Nemanič, Asst. Prof. Paul McGuiness, Asst. Prof. Miha Čekada
- Biomedical Applications of Atmospheric Pressure Plasma Technology COST MP1101
- EC; COST Office, Brussels, Belgium
- Asst. Prof. Uroš Cvelbar
- Thermal Cycle (1h at 150°C) with Outgassing Data recorded by QMS with Final SRG Measurements at R.T. PO 450274913, 2.12.11
- Dr. Vincenc Nemanič
- Outgassing Measurements of Glass Plates at Elevated Temperatures PO 450233251, 3.8.2011 Dr. Vincenc Nemanič
- 10. Characterization of Microorganism Structures by Advanced Analytical Techniques BI-ME/10-11-1

Dr. Zoran Vratnica, Institute of Public Health, Podgorica, Montenegro Prof Miran Mozetič

11. Sterilization of Medicine Materials with Gaseous Plasma BI-ME/10-11-3

Dr. Danijela Vujošević, Institute of Public Health, Podgorica, Montenegro Asst. Prof. Uroš Cvelbar

12. Interaction of Highly Dissociated CO2 Plasma with Materials Suitable as Outer Protective Layers of Future Space Vehichles PROTEUS 2010 - 2011

BI-FR/10-11-PROTEUS-005

Dr. Marianne Balat-Pichelin, Processes, Materials and Solar Energy Laboratory (PROMES-CNRS), Font-Romeu Odeillo, France

- Asst. Prof. Alenka Vesel 13. Improvement of Adhesive Properties of Biomedical Materials by Plasma Treatment BI-HR/10-11-020
  - Dr. Morana Jaganjac, Ruđer Bošković Institute, Zagreb, Croatia Asst. Prof. Alenka Vesel
- 14. Plasma Synthesis and Application of Nanowalls
- BI-JP/11-13-001

Prof. Makoto Sakine, Plasma Nanotechnology Research Centre, Graduate School of Engineering, Nagoya University, Nagoya, Japan Asst. Prof. Uroš Cvelbar

- 15. Determination of Interdiffusion Coefficients in Nano-layered Structures by High **Resolution Depth Profiling** BI-CN/11-13-006
  - Prof. Jiang Yong Wang, Shantou University, Department of Physics, Shantou Guangdong, China
- Asst. Prof. Janez Kovač 16. Plasma Synthesis and Deposition of Quantum Dots
- BI-CN/11-13-005 Asst. Prof. Xiaoxia Zhong, Shanghai Jiao Tong University, Shanghai, China
- Asst. Prof. Uroš Cvelbar
- 17. Quantum Dots for Solar Cells BI-CN/09-11-003
  - Dr. Xiaoxia Zhong, Shanghai Jiao Tong University, Shanghai, China Asst. Prof. Uroš Cvelbar
- 18. Plasma Diagnostics for Applied Research of Dusty Plasmas with Nanoparticles BI-KR11-12-001
- Prof. Choe Wonho, Korea Advance Institute of Science and Technology, Dept. of Physics / Dept. of Nuclear & Quantum Eng., Daejeon, Korea Asst. Prof. Uroš Cvelbar
- 19. Investigation of Microwave Discharges Applicable in Biomedicine and Nanotechnology BI-HU/11-12-001

Dr. Kinga Kutasi, Research Institute for Solid State Physics Optics, Budapest, Hungary Prof. Miran Mozetič

- 20. Dissociation Kinetics in Technological Plasmas BI-SR/10-11-001 Prof. Zoran Petrovič, Institute of Physics, Belgrade - Zemun, Serbia
  - Prof. Miran Mozetič
- 21. Nanowires for Photoelectrochemical Energy Conversion and Water Splitting BI-US/11-12-007

Prof. K. Mahendra Sukara, Oddelek za kemijsko inženirstvo, University of Louisville, Conn Center for Renewable Energy Research, Louisville, KY, USA Asst. Prof. Uroš Cvelbar

22. Thermoionic Energy Conversion BI-US/09-12-021

Prof. Robert Nemanich, Arizona State University, (ASU), Tempe, Arizona, USA Dr. Vincenc Nemanič

# **R &D GRANTS AND CONTRACTS**

- 1. Use of Nanoparticles as Additives in Lubricants and in Tribology Prof. Maja Remškar
- 2. Organic-inorganic thin film structures for electronic components Asst. Prof. Janez Kovač
- Development of treatments and procedures for improvement of hemocompatibility of 3. polyethylenetereftalate surfaces Prof. Miran Mozetič
- A study of plasma parameters for conditioning of the inner surfaces of a fusion reactor 4 Prof. Miran Mozetič
- 5. Printed passive electronic components for smart packaging Asst. Prof. Alenka Vesel
- Investigation of gaseous diascharges for introduction of new environmental friendly technology for functionalization of semiproduct in capacitor production 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 9 Dr. Vincenc Nemanič
- 10. Multifunctional nanocomposite coatings and paints Prof. Miran Mozetič
- 11. Research and development of integrated overvoltage protection devices based on gaseous discharger toward a reliable miniature technical solution Dr. Vincenc Nemanič
- 12. Development of advanced processes for attending high efficient nano modified textile materials Dr. Igor Mozetič
- Multifunctional Nanostructured Films for Artificial Implants Corrosion and Tribo-13 corrosion Processes
- Dr. Darinka Kek Merl 14. Synthesis of nanowires for regenerative energy cells
- Asst. Prof. Uroš Cvelbar
- Colour, absorption and protective nanolayer coatings for aluminium alloy 15. Dr. Peter Panjan
- 16. Plasma treatment of vascular grafts Prof. Miran Mozetič
- 17. Functionalization of biomedical samples by thermodynamic non-equilibrium gaseous plasma
- . Prof. Miran Mozetič 18. Toward ecologically benign alternative for cleaning of delicate biomedical instruments Asst. Prof. Alenka Vesel
- Studa of gaseous deuterium retention and release from metals relevant to ITER Dr. Bojan Zajec
- 20. Preparation of hemocompatible polymeric surfaces for biomedical applications Dr. Ita Junkar

## **RESEARCH PROGRAMS**

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

# **MENTORING**

#### Ph. D. Theses

- Gorazd Golob, Elastomer surface energy modification applying oxygen and nitrogen 1. plasma treatment with laser deactivation of the surface (mentors Mladen Lovreček, Miran Mozetič).
- Tjaša Vrlinič, Development of new anti-bioadhesive surfaces for specific neurodegenerative agents (mentor Miran Mozetič; co-mentor Fabienne Poncin-Epaillard)

# VISITORS FROM ABROAD

- Dr. Slobodan Miloševič, Marijan Biščan, dr. Nikša Krstulovič, Zlatko Kregar, Krešimir 1. Salamon, Institute of Physics, Zagreb, Croatia, several times Dr. Primož Eiselt, dr. Peter Ziegler, dr. Heinz Schmidt, Plasmabull, Lebring, Austria,
- 2. several times
- 3. Dr. Zoran Vratnica, dr. Danijela Vujoševič, dr. Ljubica Terić, dr. Sanja Medenica, prof. dr. Boban Mugoša, Institute of public health, Podgorica, Montenegro, several times
- 4 Ludvik Kumar, Kolektor Group, Idrija, Slovenia, several times
- Prof. dr. Karin Stana Kleinschek, prof. dr. Simona Strnad, Institute of textiles University 5. of v Maribor, Slovenia, several times
- Dr. Nevena Puač, dr. Željka Nikitović, Institute of Physics, Belgrade, Serbia, several times 6.
- Prof. dr. Zoran Petrović, Institute of Physics, Belgrade, Serbia , 9-12 Jan. 2011 8. Dr. Lidija Mrakovčič-Milković, dr. Ana Cipak Gašparović, dr. Morana Jaganjac, Rudjer
- Bošković Institute, Zagreb, Croatia, several times

- 9. Dr. Visakh P.M. Puthanpurachkanchira, Univerza Mahatma Gandhi, Indija, 1 May 1 Jun. 2011
- 10. Prof. Francesco Tabares, dr. Jose Fereira, Institut CIEMAT, Madrid, Spain, 11-24 Aug. 2011
- Prof. Robert J. Nemanich, North Carolina State University, Raleigh, USA, 8-13 Sept. 2011
   Prof. dr. Xiaoxia Zhong, Yi Lu, prof. Yiada Wu , prof. Ning Xu, Univerza Jiao Tong,
- Shanghai, Shanghai, IÕ-16 Sept. 2011
  Prof. dr. Masaru Hori, prof. dr. Hiroki Kondo, prof. dr. Mineo Hiramatsu, prof. dr. Makoto Sekira, University in Nagoya, Nagoya, Japan, 9-13 Sept. 2011

## STAFF

#### Researchers

- 1. Asst. Prof. Uroš Cvelbar
- 2. Asst. Prof. Janez Kovač
- 3. Prof. Miran Mozetič, Head
- 4. Dr. Vincenc Nemanič
- Asst. Prof. Alenka Vesel
   Dr. Bojan Zajec

#### Postdoctorial associates

#### 7. Dr. Aleksander Drenik

#### 8. Dr. Ita Junkar

#### Postgraduates

9. Kristina Eleršič, B. Sc.

#### 10. Gregor Filipič, B. Sc.

- 11. Gregor Jakša, B. Sc.
- 12. Metod Kolar\*\*
- 13. Martina Modic, B. Sc.

# BIBLIOGRAPHY

#### ORIGINAL ARTICLES

- 1. Andrew Das Arulsamy, Zlatko Kregar, Kristina Eleršič, Martina Modic, Uma Shankar Subramani, "Polarization induced water molecule dissociation below the first-order electronic-phase transition temperature", *PCCP. Phys. chem. chem. phys. (Print)*, vol. 13, no. 33, pp. 15175-15181, 2011.
- 2. Marianne Balat-Pichelin, Alenka Vesel, Miran Mozetič, "Microwave discharge as an effective tool for surface treatment of small samples", *IEEE trans. plasma sci.*, vol. 39, no. 11, part 1, pp. 2064-2065, 2011.
- 3. Maria Calafat, Pavel Yuryev, Aleksander Drenik, Aref Slim, Richard Clergereaux, "Carbon nanoparticle/hydrogenated amorphous carbon composite thin films formed in ECR plasma", *Plasma processes polym.* (*Print*), vol. 8, no. 5, pp. 401-408, 2011.
- 4. Uroš Cvelbar, "Removal of a thin hydrogenated carbon film by oxygen plasma treatment", *Mater. tehnol.*, vol. 45, no. 3, pp. 179-183, 2011.
- Uroš Cvelbar, "Towards large-scale plasma-assisted synthesis of nanowires", J. phys., D, Appl. phys., vol. 44, pp. 174014-1-174014-9, 2011.
- 6. Uroš Cvelbar, Ita Junkar, Martina Modic, "Hemocompatible poly(ethylene terephthalate) polymer modified via reactive plasma treatment", In: Proceedings of the 7th International Conference on Reactive Plasmas, 28th Symposium on Plasma Processing, 63rd Gaseous Electronics Conference, Paris, *Jpn. J. Appl. Phys.*, vol. 50, no. 8, pp. 08JF02-1-08JF02-5, 2011.
- 7. Aleksander Drenik, Kristina Eleršič, Martina Modic, Peter Panjan, "Probability of recombination and oxidation of O atoms on a-C:H", *Mater. tehnol.*, vol. 45, no. 3, pp. 281-285, 2011.
- Aleksander Drenik, Alenka Vesel, Arkadi Kreter, Miran Mozetič, "Recombination of hydrogen atoms on fine-grain graphite", *Appl. surf.* sci., vol. 257, no. 13, pp. 5820-5825, 2011.
- Aleksander Drenik, Pavel Yuryev, Richard Clergereaux, "Trajectories of dust particles in low-pressure magnetized plasma", *IEEE trans. plasma sci.*, vol. 39, no. 11, part 1, pp. 2734-2735, 2011.
- 10. Kristina Eleršič, Ita Junkar, Martina Modic, Rok Zaplotnik, Alenka Vesel, Uroš Cvelbar, "Modification of surface morphology of graphite by oxygen plasma treatment", *Mater. tehnol.*, vol. 45, no. 3, pp. 232-239, 2011.
- 11. Kristina Eleršič, Ita Junkar, Aleš Špes, Danijela Vujošević, Zoran Vratnica, Uroš Cvelbar, "Etching of bacterial capsule and cell wall by oxygen plasma afterflow", *IEEE trans. plasma sci.*, vol. 39, no. 11, part 1, pp. 2972-2973, 2011.

- Prof. Zoran Petrovič, prof. Gordana Malovič, Nikola Skoro, Maria Savič, Institute of Physics, Belgrade, Serbia 11–15 Sept. 2011
- 15. Dr. Vladimir Savić, Institute of Physics, Belgrade, Serbia, 4-8 Oct. 2011
- Dr. Kil Byoung Chai, dr. Heesoo Jung, prof. dr. Wonho Choe, Korea Advanced Institute of Science and Technology, Daegeon, Korea, 23–28 Oct. 2011
- Prof. dr. Marian Lehocky, prof. dr. Vladimir Sedlarik, prof. dr. Aleš Mraček, Pavel Kucharczy, Univerza Thomas Bata, Zlin, Czech Republic, 15–18 Nov. 2011
- 18. Prof. dr. Fabienne Poncin, Universite du Maine, Le Mans, France, 5–11 Dec. 2011
- 14. Borut Praček, B. Sc.
- 15. Gregor Primc, B. Sc.
- 16. Nina Recek, B. Sc.
- 17. Dr. Tjaša Vrlinič, left 01.11.11
- 18. Rok Zaplotnik\*\*
- 19. Marko Žumer, B. Sc.
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- 21. Tatjana Filipič, B. Sc.
- Technical and administrative staff
- 22. Ružica Bolte
- 23. Janez Trtnik

Note: \*\* postgraduate financed by industry

- Kristina Eleršič, Matevž Pičman, Nina Hauptman, Uroš Cvelbar, Miran Mozetič, "Interaction of oxygen species With graphene and pyrolyticgraphite surfaces", *IEEE trans. plasma sci.*, vol. 39, no. 11, part 1, pp. 2812-2813, 2011.
- Mojca Friškovec, Rahela Kulčar, Nina Hauptman, Alenka Vesel, Marta Klanjšek Gunde, "Svetolobna obstojnost termokromnih odtisov", *Vakuumist*, vol. 31, no. 2, pp. 9-13, 2011.
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  14. C. Ionita et al. (15 authors), "The use of emissive probes in laboratory and tokamak plasmas", In: PLASMA diagnostics 2010, Pont-a-Mousson, France, *Contrib. Plasma Phys.*, vol. 51, no. 2/3, pp. 264-270, 2011.
- 15. Ivan Jerman, Mohor Mihelčič, Dejan Verhovšek, Janez Kovač, Boris Orel, "Polyhedral oligomeric silsesquioxane trisilanols as pigment surface modifiers for fluoropolymer based Thickness Sensitive Spectrally Selective (TSSS) paint coatings", *Sol. energy mater. sol. cells*, vol. 95, iss. 2, pp. 423-431, 2011.
- Ita Junkar, Uroš Cvelbar, Marián Lehocký, "Plasma treatment of biomedical materials", *Mater. tehnol.*, vol. 45, no. 3, pp. 221-226, 2011.
- 17. P. Jyotishkumar, Jürgen Pionteck, Rüdiger Hässler, Martin George Sajeev, Uroš Cvelbar, Thomas Sabu, "Studies on stress relaxation and thermomechanical properties of poly(acrylonitrile-butadiene-styrene) modified epoxy-amine systems", *Ind. eng. chem. res.*, vol. 50, no. 8, pp. 4432-4440, 2011.
- P. Jyotishkumar, Jürgen Pionteck, Ceren Özdilek, P. Moldenaers, Uroš Cvelbar, Miran Mozetič, Sabu Thomas, "Rheology and pressurevolume-temperature behavior of the thermoplastic poly(acrylonitrilebutadiene-styrene)-modified epoxy-DDS system during reaction induced phase separation", *Soft matter*, vol. 7, issue 16, pp. 7248-7256, 2011.
- Andraž Kocjan, Simon Kovačič, Anton Gradišek, Janez Kovač, Paul J. McGuiness, Tomaž Apih, Janez Dolinšek, Spomenka Kobe, "Selective hydrogenation of Ti-Zr-Ni alloys", *Int. j. hydrogen energy*, vol. 36, issue 4, pp. 3056-3061, 2011.
- 20. Janez Kovač, "Surface characterization of polymers by XPS and SIMS techniques", *Mater. tehnol.*, vol. 45, no. 3, pp. 191-197, 2011.
- Zlatko Kregar, Marijan Bišćan, Slobodan Milošević, Alenka Vesel, "Monitoring oxygen plasma treatment of polypropylene with optical emission spectroscopy", *IEEE trans. plasma sci.*, vol. 39, n. 5, pp. 1239-1246, 2011.
- 22. Zlatko Kregar, Alenka Vesel, Slobodan Milošević, "Optical emission from oxygen plasma in E and H modes", *IEEE trans. plasma sci.*, vol. 39, no. 11, part 1, pp. 2502-2503, 2011.

- 23. Pavel Kucharczyk, Ida Poljanšek, Vladimír Sedlarik, Vera Kasparkova, Alexandra Salakova, Jan Drbohlav, Uroš Cvelbar, Petr Saha, "Functionalization of polylactic acid through direct melt polycondensation in the presence of tricarboxylic acid", *J. appl. polym. sci.*, vol. 12, no. 2, pp. 1275-1285, 2011.
- 24. Roman Kunič, Mohor Mihelčič, Boris Orel, Lidija Slemenik Perše, Aleš Bizjak, Janez Kovač, Stefan Brunold, "Life expectancy prediction and application properties of novel polyurethane based thickness sensitive and thickness insensitive spectrally selective paintcoatings for solar absorbers", *Sol. energy mater. sol. cells*, vol. 95, no.11, pp. 2965-2975, 2011.
- Paul J. McGuiness, Miha Čekada, Vincenc Nemanič, Bojan Zajec, Aleksander Rečnik, "Hydrogen permeation through TiAlN-coated Eurofer '97 steel", *Surf. coat. technol.*, vol. 205, no. 8/9, pp. 2709-2713, 2011.
- 26. Momir Milosavljević, Velimir Milinović, Dalibor Peruško, A. Grce, Milica Stojanović, D. Pjević, Miodrag Mitrić, Janez Kovač, K. P. Homewood, "Stability of nano-scaled Ta/Ti multilayers upon argon ion irradiation", *Nucl. instrum. methods phys. res., B Beam interact. mater. atoms*, vol. 269, no. 19, pp. 2090-2097, 2011.
- 27. Tamilselvan Mohan, Rupert Kargl, Aleš Doliška, Alenka Vesel, Stefan Köstler, Volker Ribitsch, Karin Stana-Kleinschek, "Wettability and surface composition of partly and fully regenerated cellulose thin films from trimethylsilyl cellulose", *J. colloid interface sci.*, vol. 358, iss. 2, pp. 604-610, 2011.
- 28. Miran Mozetič, "Characterization of extremely weakly ionized hydrogen plasma with a double langmuir probe", *Mater. tehnol.*, vol. 45, no. 5, pp. 457-462, 2011.
- Miran Mozetič, "Extremely non-equilibrium oxygen plasma for direct synthesis of metal oxide nanowires on metallic substrates", *J. phys., D, Appl. phys.*, vol. 44, no. 17, pp. 174028-1-174028-9, 2011.
- 30. Miran Mozetič, Alenka Vesel, Daniel Alegre, Francisco L. Tabarés, "Destruction of methane in low-pressure, electrodeless radio frequency plasma on quartz walls", *J. appl. phys.*, vol. 110, no. 5, pp. 053302-1053302-10, 2011.
- 31. Miran Mozetič, Zoran Vratnica, "Destruction of Bacillus stearothermophilus bacteria by weakly ionized low pressure cold oxygen plasma", In: Proceedings of the Salamanca-2010, 11th European Vacuum Conference, EVC-11, 8th Iberian Vacuum Meeting, IVM-8, 6th European Topical Conference on Hard Coatings, Salamanca, Spain, Vacuum, vol. 85, no. 12, pp. 1080-1082, 2011.
- 32. Vincenc Nemanič, Bojan Zajec, Marko Žumer, Corneliu Porosnicu, Cristian P. Lungu, "Hydrogen permeability of beryllium films prepared by the thermionic vacuum arc method", In: Proceedings of the 26th SOFT 2010, 26th Symposium on Fusion Technology, Porto, Portugal, *Fusion Eng. Des.*, vol. 86, no. 9/11, pp. 2421-2424, 2011.
- 33. N. T. Panagiotopoulos, Janez Kovač, Miran Mozetič, P. Patsalas, Georgios A. Evangelakis, "Formation of tetragonal or monoclinic ZrO<sub>2</sub> coatings by oxygen plasma treatment of Zr<sub>74.7</sub>Cu<sub>19.7</sub>Nb<sub>5.6</sub> glassy thin films", *J. vac. sci. technol., A, Vac. surf. films*, vol. 29, no. 5, pp. 051303-1-051303-6, 2011.
- 34. Gregor Primc, Rok Zaplotnik, Alenka Vesel, Miran Mozetič, "Microwave discharge as a remote source of neutral oxygen atoms", *AIP advances*, vol. 1, no. 2, pp. 022129-1-022129-11, 2011.
- 35. Michal Sedlacik, Vladimir Pavlinek, Marián Lehocký, Aleš Mraček, Ondrej Grulich, Petra Svrcinova, Petr Filip, Alenka Vesel, "Plasmatreated carbonyl iron particles as a dispersed phase in magnetorheological fluids", *Colloids surf., A Physicochem. eng. asp.*, vol. 387, no. 1/3, pp. 99-103, 2011.
- 36. Vladimír Sedlarik, Alenka Vesel, Pavel Kucharczyk, Pavel Urbánek, "A novel approach for qualitative determination of residual tin based catalyst in poly(lactic acid) by X-Ray photoelectron spectroscopy", *Mater. tehnol.*, vol. 45, no. 3, pp. 213-216, 2011.
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- Alenka Vesel, "Activation of polymer polyethylene terephthalate (PET) by exposure to the Co<sub>2</sub> and O<sub>2</sub> plasma", *Mater. tehnol.*, vol. 45, no. 2, pp. 121-124, 2011.
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- 40. Alenka Vesel, Aleksander Drenik, Miran Mozetič, "Evropski sončni center Font Romeu", *Vakuumist*, vol. 31, no. 3, pp. 8-11, 2011.
- Alenka Vesel, Miran Mozetič, Marianne Balat-Pichelin, "Absorption of microwave power in nitrogen plasma at moderately low pressure", *Inf. MIDEM*, vol. 41, no. 1, pp. 18-21, 2011.

- 42. Alenka Vesel, Miran Mozetič, Aleksander Drenik, Marianne Balat-Pichelin, "Dissociation of  $CO_2$  molecules in microwave plasma", *Chem. phys.*, vol. 382, no. 1/3, pp. 127-131, 2011.
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- 44. Alenka Vesel, Miran Mozetič, Peter Panjan, Nina Hauptman, Marta Klanjšek Gunde, Marianne Balat-Pichelin, "Interaction of hydrogen plasma with carbon-tungsten composite layer", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, *Nucl. Eng. Des.*, vol. 241, no. 4, pp. 1255-1260, 2011.
- 45. Alenka Vesel, Miran Mozetič, Simona Strnad, "Improvement of adhesion of fucoidan on polyethylene terephthalate surface using gas plasma treatments", In: Proceedings of the Salamanca-2010, 11th European Vacuum Conference, EVC-11, 8th Iberian Vacuum Meeting, IVM-8, 6th European Topical Conference on Hard Coatings, Salamanca, Spain, *Vacuum*, vol. 85, no. 12, pp. 1080-1082, 2011.
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#### PATENT

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# DEPARTMENT OF SOLID STATE PHYSICS

F-5

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 (2D) dimensional nuclear magnetic resonance (NMR) and relaxation, as well as quadrupole (NQR) resonance and relaxation,
- Multi-frequency NMR in superconducting magnets of 2T, 6T and 9T, as well as the dispersion of the spin-lattice relaxation time T<sub>1</sub> via field cycling,
- Nuclear double resonance and quadrupole double resonance such as <sup>17</sup>O-H and <sup>14</sup>N-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<sup>-2</sup> Hz to 10<sup>9</sup> 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 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 2011, 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"

The research of the program group Magnetic Resonance and Dielectric Spectroscopy of Smart New Materials has 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 the investigations was to discover basic laws of physics governing the behaviour of these systems, which represent a link between perfectly ordered crystals, on the one hand, and amorphous matter, soft condensed matter and living systems, on the other. The knowledge provides the key to the understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of new, multifunctional materials and nanomaterials for new applications.



Prof. Igor Muševič

In 2011, the investigations were directed to the following research fields:

#### Quasicrystals and complex metallic alloys

The tetragonal  $\sigma$  phase and the hexagonal (*hex*) phase in the Mn-Si-V(Cr) transition-metal alloy systems are stable approximant phases of a dodecagonal (12-fold) quasicrystal that can be prepared in bulk quantities. We have synthesized samples of the  $\sigma$  and *hex* phases of the composition  $Mn_{76}Si_{18}Cr_6$  and determined their magnetic

The group has investigated important open issues in the physics of unconventional superconductivity in strongly correlated electron systems, the physics of magnetically frustrated systems, the magnetism of dodecagonal approximant phases and transport phenomena in heavy-fermion conductors. The group has also discovered novel multiferroic-, relaxorand liquid-crystalline materials and developed and optimized techniques for the detection of explosives, drugs and pharmaceutical substances by magnetic resonance methods.



spins in the dodecagonal approximant phase in Mn-Si-Cr.



Figure 2: (a) Disappearance of the muon polarization at t = 0 results from a graduate spin freezing in CuNCN below 80 K. (b) Temperature dependence of the frozen-spin fraction reveals an unusually broad region of the inhomogeneous phase.

properties. In  $\sigma$ -Mn<sub>76</sub>Si<sub>18</sub>Cr<sub>6</sub>, a spin-freezing transition to a canonical spin glass phase was detected below  $T_f \approx 8$  K, characterized by a maximum in the zero-field-cooled susceptibility, a frequency-dependent cusp in the ac susceptibility, M(H) hysteresis and ultraslow time decay of the thermoremanent magnetization. In contrast, no spin glass transition was observed in the hex-Mn<sub>76</sub>Si<sub>18</sub>Cr<sub>6</sub> phase down to the lowest investigated temperature of 2 K. The analysis of the susceptibility has shown that the coupling of spins in both phases is antiferromagnetic (AFM), but the coupling strength is considerably stronger in the  $\sigma$  phase. Since both phases are structurally described by the triangle-square tiling scheme related to that of the dodecagonal quasicrystal, which imposes geometric frustration of the AFM-coupled spins on triangles, the absence of a spin-glass transition in the hex-Mn<sub>76</sub>Si<sub>18</sub>Cr<sub>6</sub> could be due to the shifting of this transition below the lowest temperature of our experimental setup, as a consequence of weaker spin coupling and the smaller moment sizes in the hex phase. In both investigated samples, tiny

 ${\rm Mn_3O_4}$  inclusions that undergo a transition to a ferrimagnetic phase at  $T_{\rm C} \approx 42$  K were detected in the magnetic signal. Geometric frustration of the interactions between the AFM-coupled spins placed at the vertices of the triangle-square tiling should be a general feature of dodecagonal quasicrystals and their approximants, so that spin-glass-type ordering is expected to occur quite commonly in the dodecagonal phases. The work was published in Kashimoto et al., Phys. Rev. B 84, 224201(2011).

#### Geometrical frustration on triangular lattices

The geometrical frustration of spin lattices leads to exotic collective magnetic ground states. A. Zorko and collaborators from Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France investigated the ground state and magnetic excitations of a triangular lattice of triangles, realized in Ba<sub>2</sub>NbFe<sub>2</sub>Si<sub>2</sub>O<sub>14</sub>. This spin-5/2 iron system features a unique single-domain, double-chiral ground state (triangular chirality of the order on each triangle and helicity of the order between planes). Employing inelastic neutron scattering they have discovered an unprecedented dynamical signature of the chiral ground state - a magnetic excitation branch that is completely chiral in the whole energy range. The paper was published in M. Loire et al., Phys. Rev. Lett. 106, 207201 (2011). Using electron spin resonance they have also unveiled the microscopic mechanism responsible for the selection of the ground state in this system. The discovery was published in A. Zorko et al., Phys. Rev. Lett. 107, 257203 (2011). A. Zorko and coworkers from IJS in collaboration with Institute of Inorganic Chemistry, RWTH Aachen University, Aachen, Germany also investigated the ground state of the spatially anisotropic triangular lattice CuNCN. In this novel quantum spin system, the magnetism is surprisingly suppressed. Local-probe studies including muon spin relaxation, electron spin resonance and nuclear magnetic resonance have shown that magnetic ordering is missing in this system down to the lowest experimentally accessible temperatures and that the magnetism is inhomogeneous. These findings were published in A. Zorko et al., Phys. Rev. Lett. 107, 047208 (2011).

#### Superconductivity in iron-based systems

We studied the family of high-temperature, iron-based superconductors Na FeAs characterized by different sodium contents. We found that below 45 K all members of the family undergo a transition into the spin-density-wave magnetic ordered state, where the portion of the Fermi surface remains gapless. This portion is directly related to the superconducting fraction, as deduced from the bulk susceptibility under 12 K. Our findings are consistent with the theories of coexisting magnetic order and superconductivity. The work was published in M. Klanjšek et al., Phys. Rev. B 84, 054528 (2011).
#### Spin ladders and chains

M. Klanjšek with colleagues from the international collaboration of groups (IJS, University of Geneva, PSI Villingen etc.) continued to study the material  $(C_5H_{12}N)_2CuBr_4$  containing spin ladders and thus belonging to the family of one-dimensional antiferromagnets. They developed a theory that successfully captures the whole phase diagram of the material obtained from measurements of nuclear magnetic resonance, neutron diffraction and specific heat. The work was published in P. Bouillot et al., *Phys. rev. B* **83**, 054407 (2011). M. Klanjšek with colleagues from LNCMI Grenoble studied the magnetic order in the natural mineral azurite containing diamond chains of spins and thus belonging to the family of one-dimensional antiferromagnets. They focused on the region of low temperatures and high magnetic fields, between the one-third magnetization plateau and full magnetization. They found that the magnetic order is not determined by the incommensurate longitudinal correlation function as predicted by some theories. Instead, the spins order antiferromagnetically in a direction perpendicular to the magnetic field. The work was published in F. Aimo et al., *Phys. Rev. B* **84**, 012401 (2011).

#### Investigations of dielectric response of relaxors in dc bias electric fields

Changes in the dynamic processes of relaxors due to a dc bias electric field have been studied in the reduced P(VDF-TrFE), a copolymer system where relaxor-like behaviour in the crystalline part can be separated from the glassy processes in the amorphous matrix, and which is very interesting as its melting point is at about 200°C (100 degrees higher than in any previously known relaxor polymer). Strong electric field dependence of the Vogel-Fulcher temperature and the activation energy has been detected. A comparison of the results with those obtained in a classical inorganic relaxor, PLZT ceramics, revealed that the nonlinear dielectric susceptibility dominantly influences the dielectric dynamics of relaxors in dc bias electric fields. We have additionally found that even a low bias voltage effectively blocks the ac electrical conductivity of the studied copolymer. Published in V. Bobnar et al., *Phys. Rev. B* **83**, 132105 (2011).

# Investigations of the influence of preparation conditions on the dielectric behaviour of CCTO thin films

The influence of the preparation conditions on the dielectric properties of  $CaCu_3Ti_4O_{12}$  (CCTO) thin films was studied by detailed dielectric investigations in broad temperature and frequency ranges. Experimental results, obtained in various CCTO thin films prepared by chemical solution deposition, and analyses in terms of the equivalent circuit reveal that the preparation conditions govern the distinctive contributions of insulating grain boundaries and semiconducting grains in different temperature and frequency ranges. With a proper post-annealing process, a dielectric constant over 3000 was obtained in films with a thickness below 500 nm. In addition, the electrical conductivity results reveal that one-dimensional variable range hopping is the dominating transport mechanism in CCTO thin films. Published in A. Eršte et al, *J. Am. Ceram. Soc.* 94, 3900 (2011).

#### High-temperature dielectric investigations of inorganic relaxor systems

We have continued high-temperature dielectric investigations of classical inorganic relaxors, which revealed astonishing results, i.e., they contradict widely accepted dogmas on relaxor properties. The results clearly reveal that polar nanoregions do not form at the so-called Burns temperature (approx. 600 K), but are continuously formed in a broad temperature range, starting well above 800 K. Furthermore, a detailed analysis of the critical behaviour undoubtedly shows that the mean-field description, used up to now, can be rejected with a high level of confidence. Published in (invited paper) V. Bobnar et al., *IEEE Trans. Ultrason. Ferroelectr. Freq. Control* 58, 2270 (2011).

#### Study of nanostructural materials and materials with large electrocaloric and thermomechanical effects

By using high-resolution calorimetry we show, via direct measurements, that the electrocaloric responsivity is maximal in the vicinity of the critical point in bulk perovskite relaxors (Figure 4) and that a secondary pyroelectric effect significantly enhances the electrocaloric response. These findings are important for the future engineering of enhanced electrocaloric materials. In a book chapter we show how to influence the thermomechanical response of the liquid crystal elastomers by changing the crosslinker density and the crosslinking temperature. We continue with the experimental and theoretical research of the liquid crystal third blue phase stabilization in a broad temperature range by the addition of the functionalized nanoparticles. Results have been published in 17 articles in international scientific journals.



Figure 3: Dielectric constant of CCTO thin films as a function of the temperature and frequency: experimental results (left) and response modelled in terms of the equivalent electrical circuit (right).



Figure 4: Electric-field and temperature dependence of the electrocaloric responsivity in the vicinity of the critical point.



Figure 5: Structure of  $CsH_5(PO_4)_2$ 



*Figure 6: Temperature dependencies of the spinlattice relaxation times of all three samples at a Larmor frequency 100 MHz.* 

#### Hydrogen-storage materials

As a part of the investigations of hydrogen-storage materials, we have studied the Ti-Zr-Ni system, where it was discovered, that the atomic ratios influence the hydrogen-absorption properties. Although these systems typically absorb around 1.5 mass % of hydrogen, we found a so-called "zero zone" area in the phase diagram, where the absorption is essentially zero. An analysis revealed that the surface oxide layer in the samples from the zero zone is significantly thicker in comparison to the samples outside the zone. By means of nuclear magnetic resonance, we have demonstrated that the electron density of state does not differ between both types of samples, therefore the differences in the electronic structure cannot account for the different oxide layer formation. The work was published in A. Kocjan et al., *Int. J. Hydrogen Energy.* **36**, 3056 (2011).

#### Superionic conductors

We have studied hydrogen dymamics in caesium pentahydrogen diphosphate,  $CsH_5(PO_4)_2$ . Our goal was to find out why this particular system does not enter the superprotonic phase upon heating, in contrast to many related compounds that exhibit such a phase. The analysis of spinlattice relaxation time revealed activatione energies for different dynamic processes in the crystal (hydrogen hopping between hydrogen bonds and hydrogen hopping, assisted by PO<sub>4</sub> tetrahedra rotations). Because of the peculiar structure, the crystal melts upon heating even before the superprotonic phase appears. Published in A. Gradišek et al., *J. Phys. Condens. Matter.* **23**, 085901 (2011).

#### NMR studies of liquid crystals

We have investigated the effects of chiral molecules on molecular dynamics to the model 5CB liquid crystal. We have measured the temperature and frequency dependence of the spin-lattice relaxation time using a superconducting and fast field-cycling magnet. Three systems were studied: pure 5CB, pure chiral 5CB\*, and a mixture of 12% 5CB\* in 5CB. The analysis revealed the changes in the molecular dynamics after the addition of chiral molecules (Figure 6). In the isotropic phase, there are two mechanisms contributing to the relaxation – molecular rotations and self-diffusion. In the nematic phase, these two processes are joined by fluctuations of the order parameter. After the addition of chiral molecules, another mechanism takes effect, namely rotations mediated by translational displacements along the helical axis. The correlation time for this motional process can be connected to the helical pitch of the system that can be independently determined using polarizing optical microscopy. Published in P. J. Sebastiao, *J. Phys. Chem. B* **115**, 14348 (2011).

#### NMR double-resonance studies of organic compounds

In 2011 we studied organic ferroelectrics and antiferroelectrics, hydrogen bonds and pharmaceutical substances. We published two papers related to organic ferroelectrics and antiferroelectrics. In the paper entitled "<sup>17</sup>O NQR and <sup>13</sup>C NMR study of hydrogen bonded ferroelectric croconic acid" (J. Seliger, J. Plavec, P. Šket, V. Žagar, R. Blinc, Phys. Status Solidi B 248, 2091-2096 (2011)) we report on the results of an NQR study of proton order in hydrogen bonds O-H...O in croconic acid,

an organic ferroelectric with the largest spontaneous polarization known till now. In the second paper entitled "A 14N nuclear quadrupole resonance study of phase transitions and molecular dynamics in hydrogen-bonded organic antiferroelectrics 55DMBP-H2ca and 1,5-NPD-H2ca" (J. Seliger et al. Phys. Chem. Chem. Phys., 2011, 13, 9165-9172), prepared together with prof. Tetsuo Asaji from Tokyo and his coworkers, we investigated antiferroelectric phase transitions in two binary hydrogen-bonded organic antiferroelectrics where chloranilic acid is the hydrogen bond donor whereas bipyridine and naphthyridine are the hydrogen-bond acceptors. We measured the proton order parameter in the bifurcated hydrogen bonds and studied a conformational exchange in bipyridine. In 3,5-pyridine dicarboxylic acid we have by 14N 17O in 2H NQR investigated the short N...H...O hydrogen bond where a phonon-driven proton transfer occurs. We determined the proton position in the hydrogen bond as a function of the temperature. The results are published in the paper entitled "Phonon-Driven Proton Transfer in 3,5-Pyridine Dicarboxylic Acid Studied by <sup>2</sup>H, <sup>14</sup>N, and <sup>17</sup>O Nuclear Quadrupole Resonance" (J. Seliger, V. Žagar, J. Phys. Chem. A 2011, 115, 11652-11656). In a review paper entitled "Nuclear Quadrupole Resonance Study of Hydrogen Bonded Solid Materials" (J. Seliger, Acta Chim. Slov. 2011, 58, 471-477)) we report on the 170 and 14N NQR studies of hydrogen bonds and on the correlations observed between the structural and NQR parameters. We investigated two pharmaceutical substances by clioquinol and cloxiquine NQR. In the paper entitled "Supramolecular synthon pattern in solid clioquinol and cloxiquine (APIs of antibacterial, antifungal, antiaging and antituberculosis drugs) studied by <sup>35</sup>Cl NQR, <sup>1</sup>H-<sup>17</sup>O and <sup>1</sup>H-<sup>14</sup>N NQDR and DFT/QTAIM" (J. N. Latosińska et al. J. Mol. Model 2011, 17, 1781-1800) we together with dr. Jolanta Latosinska and her coworkers from Poznan report on the study of these compounds by NOR and quantum chemical calculations in relation to the differentiation between crystal polymorphs and to the study of intermolecular hydrogen bonds.

#### NQR excitation sequences for portable devices

Nuclear quadrupole resonance has a great potential for applied use. Its main advantages are: the technique is non-invasive, has a big specificity for the identification of various solid materials and requires relatively simple equipment, especially when compared to nuclear magnetic resonance. The biggest element which is required for standard NQR operation is the RF amplifier, with typical powers of 500 W for small coils and up to 10 kW for very large coils. To reduce the size and power requirements of this element, and thus increase portability, we have been developing several techniques of non-standard excitation. The most effective method found so far is excitation with WURST pulses, which require up to 100 times less power than conventional rectangular pulses. We have experimentally demonstrated the efficiency of the sequence by using only 2.5 W for a successful detection of the explosive TNT with <sup>14</sup>N NQR. Published in A. Gregorovič et al., J. Mag. *Res.* 209, 79 (2011).

#### New method for synthesizing Au nanoparticles

A new method of synthesizing nanoparticle-functionalized nanostructured materials via Aerosol-Assisted Chemical Vapour Deposition has been developed. The co-deposition of Au nanoparticles with WO, nanoneedles has been used to deposit a sensing layer directly onto gas sensor substrates providing devices with a six-fold increase in the response to low concentrations of ethanol (1.5 ppm at °C). Published in S. Vallejos et al., Chemical Communications 47, 565(2011).

#### Nanoscale spectroscopy with polarized X-rays by NEXAFS-TXM

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 this work, we described a full-field transmission X-ray microscope (TXM) that generates high resolution, large-area NEXAFS data with a collection rate that is two orders of magnitude faster than is possible with STXM. The TXM optical design combines a spectral resolution of E/DE5 13104 with a spatial resolution of 25 nm in a field of view of 15–20 mm and a data acquisition time of  $\sim$ 1 s (Figure 9). As an example, 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. This was recognized by the editors of Nature Photonics, who accepted the paper entitled "Nanoscale spectroscopy with polarized X-rays by NEXAFS-TXM" for publication.

#### Liquid-crystalline elastomers

A new type of liquid single-crystal elastomer forming a chiral smectic A\* phase has been prepared using chiral lactic acid derivative as a comonomer. This elastomer possess orthogonal paraelectric SmA\* and ferroelctric SmC\* phases over a broad temperature interval. We also synthesized and characterized composites of liquid single-crystal elastomers and MoO<sub>3,x</sub> nanowires, homogeneously distributed across the surface of the soft matrix. We have demonstrated that, using a conventional two-step polymerization approach, the nanowires are preferentially aligned along the nematic director. Published in V. Domenici et al., J. Mater. Sci. 46, 3639 (2011).

#### Polymer dynamics studied by NMR

The velocity autocorrelation spectrum of the polybutadiene polymer segmental motion has been worked out according to the Rouse and the tube/reptation model to compare it to the experimental results obtained by the new NMR modulated gradient spin-echo method. The analysis of Figure 9: Workflow for NEXAFS-TXM polybutadiene shows the segmental autocorrelation spectrum typical for the reptation-like motion *measurements*. of a polymer in a "tube". Published in *Macromol. Symp.* 305, 55(2011).





Figure 7: <sup>14</sup>N NQR spectra of the explosive TNT when detected with 2.5 W of RF power. The full spectrum is excited with WURST pulses (dashed line), whereas only a partial excitation is achieved with standard, rectangular pulses (solid line).



Figure 8: HRTEM images of (a) WO, nanoneedle with Au nanoparticles on the surface and (b) closeup of Au nanoparticles.

#### 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

In 2011, an important achievement was the discovery of knots and links in chiral nematic colloids. The group has investigated skyrmion defects in liquid-crystal blue phases, studied the stabilization of blue phases by colloidal dispersion, and has investigated the topological properties of nematic braids. Members of the group have also investigated a ciliary beating pattern, analysed the optical properties of exfoliated MoS<sub>2</sub> nanotubes and developed liquid-crystal technology.

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.

#### Knots and links in chiral nematic liquid crystals

In a paper entitled "Reconfigurable Knots and Links in Chiral Nematic Colloids", U. Tkalec et al, *Science* **333**, 62(2011), we report on an experimental observation and theoretical interpretation of knots and links in a colloidal mixture of glass microspheres in a chiral nematic liquid crystal. We have found that defect loops can spontaneously form a variety of knotted and linked structures. We have used laser tweezers to analyse the structure of these microscopic knots and links, and we could change their configuration by applying a strong and localized laser light. A theoretical approach, combing a phenomenological theory and topology has been used to explain and



Figure 10: President of the Republic of Slovenia, Dr Danilo Türk, visited J. Stefan Institute and the Soft Matter Physics Laboratory of the Solid State Physics Department on October 17, 2011. The President met and congratulated the authors of the Science paper on knots and links in liquid crystals for their success.

analyse the structure of the observed knots and links. We have observed that knots and links of arbitrary complexity could be formed in the chiral nematic colloids. Knots and links are objects studied within the mathematical discipline of mathematics, topology, and have always played an important role in human history. They were used in building, sailing, handcraft and art. The work of Tkalec et al. is not only a rare example of the realization of an abstract mathematical theory in Nature, but also has a potential practical impact. The authors are considering liquid-crystal knots and links to be used for the binding and fabrication of photonic microstructures that could control the flow of light in soft matter.

Stabilization of blue phases with dispersed colloidal particles: Modelling and simulations show that the dispersion of colloidal particles in blue phases (BPI & BP II) leads in principle to 3D colloidal crystals exhibiting the same symmetry as the underlying orientational ordering lattice. Using particles with weak surface anchoring the blue phase stability range substantially increases (Fig.SZ1). Such colloidal arrays are in fact photonic crystals that would have an advantage over pure blue phases because particles with specific optical, electric, and magnetic properties introduce possibilities for additional manipulation. Published in Ravnik et al., *Proc. Nat. Acad. Sci. U. S. A.* **108**, 5188(2011).

Skyrmion lattices in confined blue phases: We showed theoretically, with the aid of numerical methods, that a highly chiral nematic liquid crystal can accommodate a quasi-two-dimensional Skyrmion lattice as a thermodynamically stable state, when it is confined to a thin film between two parallel surfaces imposing normal align-

Figure 11: Increase of the stability range of colloidal BPI & BPII phases (red lines and circles) in comparison to pure BPI & BPII phases (black lines and circles).

ment (Fig.SZ2). A chiral nematic liquid-crystal film can thus serve as a model Skyrmion system, allowing a direct investigation of their structural properties by a variety of optical techniques at room temperatures that are far less demanding than for Skyrmion systems discussed previously in two-dimensional electron gases exhibiting the quantum Hall effect, chiral ferromagnets, and Bose–Einstein condensates. Published in J. Ichi Fukuda, S. Žumer, *Nature Communications* 2, art. no. 246(2011). We expect these soft-matter structures to be relevant for photonic applications.

**Topological invariants of nematic braids:** Coupling geometrical and topological aspects of disclination loops that are in fact ribbons with the three fold symmetry led to the introduction of a new topological invariant - self-linking number as the sum of writhe and twist. We also unveil a simple rewiring scheme for the orthogonal crossing of two 3-fold ribbon disclinations, based on

a tetrahedral rotation of two relevant disclination segments, which allows us to predict possible nematic braids and calculate their self-linking numbers. Complex nematic braids with knots and links of disclinations with three-fold symmetry that can entangle homeotropic colloidal particles in nematic and chiral nematic phases can be with this formalism completely classified. Published in S. Čopar and S. Žumer, Phys. Rev. Lett. 106, 177801 (2011).

Early-stage domain coarsening of the isotropic-nematic phase transition: We performed a Brownian molecular dynamics simulation of the early-stage domain-coarsening dynamics of the temperature-driven isotropic-nematic liquid-crystal phase transition. We show that soon after the transition a bimodal distribution of domains appears, where the shorter branch gradually vanishes. The behaviour of the system is in accordance with the predictions of the Kibble-Zurek mechanism, which was originally introduced to model conditions in the early universe. Published in Z. Bradač et al., J. Chem. Phys. 135, 024506(2011).

Finding the ciliary beating pattern with optimal efficiency: Many biological processes work with an extremely high energetic efficiency, but at first glance this does not hold for ciliary propulsion, reaching about 1%. We have re-examined the problem at the level of a single cilium and an infinite ciliated surface. We numerically determined the optimal shape of the ciliary beating pattern and showed that the optimal collective stroke is remarkably similar to that observed in microorganisms (Fig. AV1). For Paramecium we showed that the experimentally measured hydrodynamic efficiency reaches about 50% of the theoretically possible optimum. Published in N. Osterman, I. Vilfan, Proc. Natl. Acad. Sci. U. S. A. 108, 15727(2011).



Figure 12: Blue-phase skyrmion defect lattice. In red are the defect areas of depressed order, while white and grey bars denote nematic director field.



Figure 13: (a) represents a threefold disclination profile visualized using the splay-bend parameter. (b-e) are the well-known entangled dimers characterized by the self-linking number, writhe, and free-energy differences from the ground state.

sub-nanometre-thick single layers was stable for weeks. The monolayers represent an inorganic analogue of grapheme. We have evidenced the quantum-confinement effect from a shift of optical absorption peaks. The results are applicable in optics and nanoelectronics. Published in Višić et al., Nanoscale Research Letters 6, 593(2011). EU and US patents for the synthesis of tungsten- and molybdenum-based nanotubes:

Optical properties of exfoliated MoS[sub]2 coaxial nanotubes - analogues of grapheme:

We have exfoliated MoS<sub>2</sub> nanotubes for the first time. The resulting material in the shape of

A European patent was granted for the synthesis of electrically conductive nanowires of W<sub>5</sub>O<sub>14</sub> (Remškar et al. 2011). The nanowires show up to eight orders of magnitude higher conductance than the stoichiometric WO<sub>2</sub> compound and belong to photochromic materials. They represent a starting material for the synthesis of WS, nanobuds, where hollow WS, nanospheres are attached on the surface of the WS, nanotubes. In parallel a US patent was also granted for the synthesis of MoS<sub>2</sub> nanotubes and Mo<sub>2</sub>O<sub>14</sub> nanowires (Mrzel et al. 2011). The patent also protects geometry, where MoS, nanospheres are situated inside the MoS, nanotubes. The MoS, nanotubes are an excellent lubricant and added to oils and greases they decrease friction by up to 50 % and wear by up to 90 %.

#### Low-temperature STM microscopy of surfaces in a ultra-high vacuum

In the field of surface physics we are currently performing low-temperature experiments on and the corresponding calculations of the Bi and Sb (111) surfaces, which we intend to cover with sub- and mono-atomic layers of Se. Our goal is to construct very thin islands and layers of the topological insulators Bi<sub>2</sub>Se<sub>2</sub> and Sb<sub>2</sub>Se<sub>3</sub>. In 2011, we have started the construction of our first apparatus for experiments with ultra-cold atoms. Cold atoms offer an exciting possibility to study strongly correlated systems, which can be used as quantum simulators of other complicated systems, e.g., high-temperature superconductors. The one-dimensional conductor (NbSe<sub>4</sub>)<sub>10/2</sub> I was examined by x-ray diffraction and high-resolution transmission electron microscopy (HRTEM). By calculating its electronic properties and by simulation of the X-ray and electron diffraction patterns it was shown that the disorder detected is a result of a mismatch between the infinite NbSe, chains. The structural phase transition at 285 K was attributed to a Jahn-Teller distortion. Published in A. Prodan et al. Proc. 22. IUCr, Acta Cryst., 67, C512(2011). The structural relaxation around individual hydrogen atoms and their binding energies were studied for a few hydrogenated TiBx structures by means of density functional theory methods. Starting with the symmetric hydrogen sites a random structure searching has revealed all energetically stable adsorption sites. core of the defect loops and is therefore visible. Published in R. Žitko et al., Int. J. of Hydrogen Energy 36, 12268 (2011).



Figure 14: Knots are formed in the dispersion of glāss microspheres in a chiral nematic liquid crystal. The knots are formed from closed defect loops. The liquid crystal has reduced order in the



Figure 15: Optimal ciliary beating pattern. The calculated beating pattern of cilia densely covering a surface strongly resembles the dynamics of biological cilia. The stroke is asymmetric: stretched in one direction and sweeping along the surface in the other. The phases of cilia form metachronal waves.



Figure 16: Figure shows differently oriented MoS<sub>2</sub> flakes produced by the exfoliation of MoS2 nanotubes. The flakes are thinner than one nanometre.



Figure 17: HRTEM image of a (NbSe4)10/31 crystal, recorded with the electron beam parallel to the [110] direction; an overlapped corresponding simulated image and a structural model are shown in the inset.

#### Technology of optical shutters based on liquid crystals

The concept of STN LCD light shutters and their angular compensation by means of the negative c-plate birefringence (EP 1883854) has been developed at the JSI in previous years. During this year it was upgraded to allow for the simultaneous use of the small positive in-plane birefringence, the formation of which is inherent to its production process. This upgrade is the subject of a CIP patent application US 13/208,378. In 2011 USPTO also granted the patent US 8,026,998 describing the continuous variation of the protective shade with automatic LCD protective filters. The introduction of the above technical solution in the JSI's spin-off company Balder's production process allows the latter to be the only producer in the world capable of producing active LCD welding filters with the highest optical quality (1/1/1/1), as specified by the international Standard EN 379. As a result the International Standard Organization (ISO) invited the JSI and Balder to participate in its expert group (ISO/TC94/SC6/WG2 in WG4) preparing the new world Standard for Eye and Face protection. The contribution of JSI/Balder within the ISO Expert group is as follows. Draft of the ISO Standard: "Occupational Eye and Face Protection" (co-authors) has been prepared. The draft has already been approved on the first level of international verification and will be accepted in its final form at the occasion of the next ISO meeting (June 2012). A new standardization measuring process for the light sensitivity determination of automatic welding filters has been developed. The new method will be published by the German Standardization Institution "TÜV Reinland". An "artificial plasma light source" simulating TIG welding has been developed; likewise the draft ISO Standard, it will be accepted at the occasion of the next ISO meeting (June 2012) as the new ISO standard light source.

#### Detection of low levels of vapour concentration in explosives

In collaboration with the Faculty of Electrical Engineering and the Faculty of Chemistry and Chemical Technology of the University of Ljubljana, we have developed a miniature and portable device for the detection of low concentrations of the vapours of explosives. We have used a differential pair of chemically functionalized microcapacitors together with ultrasensitive and low-noise detection electronic circuits to detect 1 molecule of TNT in  $10^{+12}$  molecules of a carrier gas N<sub>2</sub>. The work was published in D. Strle et al., *IEEE Sens. J.*, in press 2011, doi: 10.1109/JSEN.2011.2168203.

# The group has been awarded two EU patents in the field of liquid-crystal-based materials and devices

In 2011 the members of the programme group have been awarded two patents from the field of materials and devices, based on liquid crystals. European patent EP 1975656B1 "Metamaterials and resonant materials based on liquid-crystal dispersions of colloidal particles and nanoparticles" authored by I. Muševič, M. Škarabot, S. Žumer and M. Ravnik is protecting the method of fabrication of composite materials made of a liquid crystal, colloidal particles and nanoparticles. In this multicomponent dispersion, the nanoparticles are trapped into the core of the disclination defect lines. The electric properties of such hierarchical structures are similar to the ring microresonators and the material exhibits a negative magnetic response, which is the property of metamaterials. The second EU patent EP 1927885B1 "Multistable liquid crystal device" by Th. Rasing, S. Lazarenko, I. Muševič, M. Škarabot and M. Uplaznik, is from the field of microconfined liquid crystals, where the nematic liquid crystal is trapped into a geometrically regular confining structure, formed by optical or electronic lithography. Because of the topological constraints of the ordering field, such a device exhibits a multitude of stable optical states. These can be addressed either by an electric field or by a strong laser light.

#### 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 the glycosaccharide matrix as well as their interactions with various materials that enter into their native environment. Novel

spectroscopic and microspectroscopic 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. Besides, we focus on medical methods of optimization, like tumour treatment methods, magnetic resonance imaging and mathematical modelling of trombolisis, magnetic resonance microscopy in forestry, wood science and food processing as well as on 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 biocompativility point of view. The recent developments in **fluorescence microspectroscopy** (FMS) enabled the acquisition of the fluorescent spectra within very small volume elements and the characterization of a local molecular environment of fluorophore molecules. FMS was applied to localize the response of the cells to the presence of various materials, especially nanomaterials used for the antimicrobial protection of the surfaces. In addition, FMS was used to unravel the interaction between the cells and macrostructured materials like medical materials. The bleaching problem was solved with a special algorithm developed to neutralize the bleaching effect in spectral analysis. The FMS system was optimized and upgraded with a system for micromanipulation to enable measurements of the force between the cells and the scaffolds.

On the segment of the **development and synthesis of various molecular probes** (nitroxides, T fluoprophors and the probes that combine both groups in the same molecule) our research was

focused on amphiphilic fluorescent probes with NBD (as an environmentally sensitive probe) inside a membrane environment to enable sensitivity to local environment (polarity). We showed sensitivity to the cholesterol concentration, but only between the gel and liquid-crystalline phases. The structure optimization of the new molecular tool opens up new opportunities in the combined exploration of the same sample with fluorescence microspectroscopy and electron paramagnetic resonance spectroscopy at the same time.

Within the research of the **interaction between** biologically active materials and cells we focused on the investigation of **cancerostatic alkylphospholid** (perifosine, OPP) with **cell membranes** using EPR spectroscopy and

an in-house developed computer program for the simulation of EPR spectra (EPRSIM). Anticancer agents OPP directly target the cell membrane but not the DNA. It shows a selective apoptotic response in tumour cells, sparing normal cells and was found to be promising for breast-cancer therapy. An antitumor effect was found for estrogen receptor negative (ER-) tumour cells (MT-3 cell line) *in vivo*, while no effect was found for receptor positive (ER+) tumour cells (MCF-7).

Spin labelled OPP (SL-OPP) was used to identify that the difference between MCF7 cells MT-3 cells in the transport of SL-OPP across the plasma membrane can be assigned to the low accumulation in MCF7 cells. Liposomal OPP formulations with a low CH concentration quickly release entrapped

spin probe when mixed with breast-cancer cells, while the release is much slower for liposomes with 50 or more mol% cholesterol. At room temperature the release is the same for MT-3 and MCF7 cells. However, at physiological

temperature the amount of released content increases for the OPP sensitive MT-3 cells, but remain in the same range for MCF7 cells. In collaboration with the Biotechnical Faculty the **membrane characteristics of a new class of liposomes prepared from dietherarcheal lipids** and their mixtures with standard dipalmitoyl-phosphatidylcholine (DPPC) lipids, we found that these two types of lipids mix well in different molar ratios and form liposomes upon hydration. Their stability decreases with a higher ratio of conventional lipids; however, new characteristics emerge. For arheosomes prepared from dietherarcheal lipids isolated from *Aeropyrum pernix* K1 grown in the medium with different pH (from pH 6 to 8) it was found that the average membrane fluidity was not influenced by the pH of the growth medium significantly.

One of our main activities is the study of membrane structuring. In this respect it is important to note that different time and distance scales of the methods can lead to very different conclusions regarding the stability of the heterogenous structure of the membranes. For an integral view one has to use an appropriate set of methods. A collaboration with foreign partners allows us to use different biophysical methods that are complementary to the methods available in our lab. So besides the method of attenuated total reflection Fourier transform infrared spectroscopy (ATR-

Publication of the article "Ferri-liposomes as an MRI-visible drug-delivery system for targeting tumours and their microenvironment" in the *Nature Nanotechnology* journal. We showed that new ferri-liposomes can be used as a very effective T2 MR contrast agent and for the targeting of therapeutic agents to a specific location in the body using an external magnetic field.



Figure 18: Image on the left. Eye-protecting helmet using an active and fast LCD shutter, produced by the JSI spin-off company Balder d.o.o. The right image shows the prototype of an artificial plasma light source, used for measuring the eye-protecting characteristics of welding filters.



Figure 19: SEM image of a differential pair of microcapacitors, fabricated in CMOS technology. The pair serves as a precise molecular detector.



Figure 20: Application of fluorescence microspectroscopy (right) enables the spectral identification of fluorescein-labelled polystyrene latex nanoparticles (50 nm diameter, violet) incubated within cancer cells labelled with lipophilic molecules with NBD dye partitioning in the membranes (green). Classic intensity image (left) can resolve membranes and particles due to substantial spectral overlap.

FTIR) we also used calorimetry and x-ray scattering to study the effect of ceramide on the structure and properties of membranes. We showed that **these complementary methods allow an efficient examination of phase diagrams of model membranes composed of different lipid mixtures**. In this way we were able to classify different types of membrane heterogeneity as stable or unstable.

To improve the **protein structure determination** based on the conformational space modelling of the protein side chains (CSM), we set-up a cluster based on 8000 graphical processor cores. Together with improved sampling methods this enabled us to confirm that the energy topology of the spin-probe conformational space is environment insensitive, i.e., not sensitive to the neighbouring amino acids as well as lipids or a water local environment. On the contrary, those conditions affect the rotational diffusion. This enables us to speed up the calculation of the restrictions in conformation spaces within the appropriate time window of the EPR spectroscopy and a simple generalization of the inverse problems in protein-structure determination.

Titanate nanomaterials generate short-lived radicals in the processes of photocatalysis, thus preventing the growth of bacteria. We synthesised titanate nanomaterials (TiNTs) with a high specific surface area and a significant antimicrobial activity. Photogeneration of primary hydroxyl radicals by TiNTs was detected in the laboratory with the electron paramagnetic resonance method with spin trapping in the presence of 30% of ethanol. The stable deposition of TiNTs on polymer surfaces was achieved even after soaking in different conditions (neutral, acid, and base) for up to six times. A reduction in the colony-forming units of non-pathogenic Listeria Innocua was observed independent of the wavelength of the illuminating light. The highest reduction was achieved at lower wavelengths on TiNTs covered surfaces.

We confirmed our assumption that **thrombolysis is not just a biochemical process** in which there is a complete degradation of fibrin, but under the influence of rapid blood flow it leads to the formation of strong mechanical forces to the surface of a blood clot that result from blood viscosity. These forces cause the breakage of large parts of the clot formed by the fibrin network and blood cells (primarily erythrocytes). These torn pieces may range in size from individual cells, to clusters of several hundred cells. With optical microscopy experiments,



Figure 21: Histological image of a venous blood clot behind a venous valve (left) and the simulation of the blood flow behind the valve (right). Simulation of the flow indicates the possibility of the occurrence of vortex flow, which may contribute to platelet activation and consequently to the formation of a blood clot. we also showed that the size of these clusters largely depends on the blood flow. In a slow stream of blood only small clusters were formed, while at a higher speed significantly larger pieces of the clot were torn. These results also explain why the thrombolysis is much faster in a faster flow than in a slow flow. The promotion of thrombolysis in the rapid blood flow is greater than expected due to better permeation of the clot with the thrombolytic agent and significantly larger forces of the streaming blood to the surface of the clot. Based on the results of this study a computer simulation of the microscopic processes of thrombolysis was developed. Its results are in good agreement with our measurements.

*lood clot.* By MRI, we monitored the **freezing dynamics of different types of vegetables** and showed the differences between rapid and slow freezing. We have shown that MR imaging is an efficient tool for monitoring the freezing process, because it can clearly distinguish between fresh and frozen food areas. MRI also

reflects the differences in NMR relaxation times and the diffusion characteristics of food before and after freezing.

**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, a knowledge of the gel layer's 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 temperature on the kinetics of medium penetration and hydrogel formation in xanthan tablets. The swelling dynamic is independent of the temperature in the range between 20°C and 40°C.



Figure 22: Series of dynamically acquired T2weighted images (in 11-min intervals) of a carrot sample undergoing slow freezing and thawing. A complete loss of the sample structure after thawing is apparent.

The+MRI contrast properties of a new contrast agent based on cobalt ferrite nanoparticles were tested. Most of the MR contrast agents based on the ferrite nanoparticles have very large r2 relaxivities, i.e., the T2 significantly shortens already at low nanoparticle concentrations, while the r1 relaxivity (the contrast agent shortens the spin-lattice (T1) relaxation time) is much lower and can therefore be only used as a negative (T2) MR contrast agent. The negative T2 effect is very strong. The MR signal diminishes in the vicinity of the presence of the contrast agent on the T2-weighted MR images and the dark region on the T2-weighted images can be confused with the dark region originating from other causes, such as calcification or metal deposits. Therefore, the contrast agent that would enable a simultaneous detection of the probe on T1-weighted and T2-weighted MR images would solve the problem. By using T1-weighted images the confusion with the dark regions originating from other causes can be excluded. The contrast properties were tested using 1% agarose with relaxation times that are similar to those of some tumour tissues. The results show that the cobalt ferrite nanoparticles can be used as positive T1 and negative T2 MRI contrast agents and their unique double T1 and T2 contrast properties could provide the possibility for their use in MRI diagnostics, both as positive and negative contrast agent.

Part of our research was focused to a study of the ability of NMR-modulated gradient spin echo (MGSE) to provide information about the **translational dynamics of polymer segments** via the measurement of segmental velocity autocorrelations. Since the method requires the formulation of dynamics in the frequency domain, at first we derived the expression for the velocity autocor-

relation spectrum (VAS) of the segmental motion according to Rouse and deGennes the tube/ reptation model. The resulting VAS can be fitted well to the results of the measurement on the samples of molten polybutadiene and polyethylene. Thus, they represent a first direct experimental verification of the snake-like motion in a "tube" of entangled polymer chains. It appears that this new understanding of macromolecular motion makes it possible to also explain the unusual results of our previous MGSE measurement of bulk water as a kind of Rouse-type motion in a network of hydrogen bonds in water. In the next study we have shown the ability of the NMR pulsed gradient spin echo to provide information about molecular self-diffusion in nanopores. The method was successfully tested on the sieve of a polyamide membrane.

The above research has been supported by a number of international projects financed by the European Union within the Fifth and Sixth Frameworks as well as NATO. It was also supported within the bilateral Slovenian–USA, Slovenian–German and Slovenian–Greek and other scientific cooperations. International cooperations with

- The high magnetic field centres in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field centre 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 für 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 2011

- A. Zorko, P. Jeglič, A. Potočnik, D. Arčon, A. Balčytis, Z. Jagličić, X. Liu, A. L. Tchougreeff, A. L. Dronskowski, Unconventional magnetism in a nitrogen-containing analog of cupric oxide. *Phys. Rev. Lett.* 107, 047208(2011).
- 2. A. Zorko, M. Pregelj, A. Potočnik, J. van Tol, A. Ozarowski, V. Simonet, P. Lejay, S. Petit, and R. Ballou, Role of antisymmetric exchange in selecting magnetic chirality in Ba<sub>3</sub>NbFe<sub>3</sub>Si2O<sub>14</sub>. *Phys. Rev. Lett.* **107**, 257203 (2011).
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- S. Kashimoto, A. Kocjan, Z. Jagličić, S. Jazbec, H. Iga, T. Ishimasa, J. Dolinšek, Magnetic properties of σ and hexagonal-Mn<sub>7</sub>Si<sub>18</sub>Cr<sub>6</sub> approximant phases of a dodecagonal quasicrystal. *Phys. Rev.* B 84, 224201(2011).
- M. Loire, V. Simonet, S. Petit, K. Marty, P. Bordet, P. Lejay, J. Ollivier, M. Enderle, P. Steffens, E. Ressouche, A. Zorko, R. Ballou. Parity-broken chiral spin dynamics in Ba<sub>3</sub>NbFe<sub>3</sub>Si<sub>20</sub>. *Phys. Rev. Lett.* **106**, 207201(2011).
- G. Mikhaylov, U. Mikac, A. A. Magneva, I. V. Itin, E. P. Naiden, I. S. Psakhye, L. Babe, T. Reinheckel, C. Peters, R. Zeiser, M. Bogyo, V. Turk, S. G. Psahkye, B. Turk, O. Vasiljeva. Ferri-liposomes as an MRI-visible drug-delivery system for targeting tumours and their microenvironment. *Nature Nanotechnology* 6, 594(2011).
- J. Fukuda, S. Žumer. Quasi-two-dimensional Skyrmion lattices in a chiral nematic liquid crystal. *Nature Com*munications 2, 5(2011)
- 8. J. Fukuda, S. Žumer. Ring defects in a strong confined chiral liquid crystal. Phys. Rev. Lett. 106, 097801(2011).



Figure 23: T1- and T2-weighted MR images of different concentrations of cobalt ferrite nanoparticles in 1% agarose.

- 9. S. Čopar, S. Žumer. Nematic braids: topological invariants and rewiring of disclinations. *Phys. Rev. Lett.* **106**, 177801(2011).
- 10. M. Ravnik, G. P. Alexander, J. M. Yeomans, S. Žumer. Three-dimensional colloidal crystals in liquid crystalline blue phases. *Proc. Natl. Acad. Sci. U. S. A.* 108, 5188(2011).
- U. Tkalec, M. Ravnik, S. Čopar, S. Žumer, I. Muševič, Reconfigurable knots and links in chiral nematic colloids. Science (Wash. D.C.) 333, 62(2011).
- 12. N. Osterman, A. Vilfan, Finding the ciliary beating pattern with optimal efficiency. *Proc. Natl. Acad. Sci. U. S. A.* 108, 15727(2011).
- 13. I. Muševič, S. Žumer. Liquid crystals : maximizing memory. Nature Materials 10, 266(2011).

#### Some outstanding publications in 2010

- 1. A.Y.Ganin, Y. Takabayashi, P. Jeglič, D. Arčon, A. Potočnik, P.J. Baker, Y. Ohishi, M.T. McDonald, M.D. Tzirakis, A. McLennan, G.R. Darling, M. Takata, M.J. Rosseinsky, K. Prassides. Polymorphism control of superconductivity and magnetism in Cs<sub>3</sub>C<sub>60</sub> close to the Mott transition. *Nature (London)* 466, 221-225(2010).
- 2. A. Zorko, B. Fabris, P. Mendels, K. Marty, P. Bordet. Ground state of the easy-axis rare-earth kagome langasite Pr<sub>3</sub>Ga<sub>5</sub>SiO<sub>14</sub>. *Phys. Rev. Lett.* **104**, 057202-1-057202-4(2010).
- B. Zalar, A. Lebar, D.C. Ailion, R.O. Kuzian, I. Kondakova, V.V. Laguta. <sup>7</sup>Li NMR Investigation of Li-Li pair ordering in the paraelectric phase of weakly substitutionally disordered K<sub>(1-x)</sub>LixTaO<sub>3</sub>. *Phys. Rev. Lett.* **105**, 226402-1-226402(2010).
- 4. E. Zupanič, R. Žitko, H. J. P. van Midden, I. Muševič, A. Prodan. Pinning of adsorbed cobalt atoms by defects embedded in copper (111) surface. *Phys. Rev. Lett.* **104**, 196102-1-196102-4(2010).
- A. Omerzu, B. Anželak, I. Turel, J. Štrancar, A. Potočnik, D. Arčon, I. Arčon, D. Mihailovič, H. Matsui. Strong correlations in highly electron-doped Zn(II)-DNA complexes. *Phys. Rev. Lett.* 104, 156804-1-156804-4(2010).
- Jun-ichi Fukuda, S. Žumer. Novel defect structures in a strongly confined liquid-crystalline blue phase. *Phys. Rev. Lett.* 104, 017801-1-017801-4(2010).
- M. Humar, I. Muševič. 3D microlasers from self-assembled cholesteric liquid-crystal microdroplets. *Opt. Express* 18, 26995-27003(2010)
- Vilfan, A. Potočnik, B. Kavčič, N. Osterman, I. Poberaj, A. Vilfan, D. Babič. Self-assembled artificial cilia. Proc. Natl. Acad. Sci. U. S. A. 107, 1844-1847(2010).
- A. Kavalenka, I. Urbančič, S. Kure, J. Štrancar. Conformational analysis of the partially disordered measles virus N<sub>(TAIL)</sub>-XD complex by SDSL EPR spectroscopy. *Biophys. J.* 98, 1055-1064(2010).

#### Patents granted

1. Metamaterials and resonant materials based on liquid crystal dispersions of colloidal particles and nanoparticles

Igor Muševič, Miha Škarabot, Slobodan Žumer, Miha Ravnik EP1975656 (B1), European Patent Office, 8.6.2011.

- Multistable liquid crystal device Theo Rasing, Sergiy Lazarenko, Igor Muševič, Miha Škarabot, Marko Uplaznik EP1927885 (B1), European Patent Office, 27.7.2011.
- Procedure for synthesis of threadlike tungsten oxide W5014 Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih EP2114827 (B1), European Patent Office, 16.2.2011.
- Process for the synthesis of nanotubes and fullerene-like nanostructures of transition metal dichalcogenides, quasi one-dimensional structures of transition metals and oxides of transition metals Aleš Mrzel, Maja Remškar, Adolf Jesih, Marko Viršek US8007756 (B2), United States Patent and Trademark Office, 30.8.2011.

#### Awards and appointments

- Andreja Jelen, Marica Starešinič: Successful participation in the "OE-A Competition for Multifunctional Demonstrators based on Organic and Printed Electronics" by submitting the demonstrator "Security Vest". Frankfurt, Germany, Organic Electronics Association (OE-A) : a working group within German Engineering Federation VDMA.
- 2. Marta Lavrič: Ferbar Prize, Ljubljana, Faculty of Education, Liquid crystal elastomers.
- 3. Igor Muševič: Mentor of the year 2011, Ljubljana, Slovenian Society of Young Researchers

#### Organization of conferences, congress and meetings

1. 11th European conference on liquid crystals (ECLC 2011), Maribor, 6. 2.-11. 2. 2011

### INTERNATIONAL PROJECTS

- 1. Light Element Molecular Superconductivity: An Interdisciplinary Approach LEMSUPER
  - 7. FP. 283214

EC; Prof. Kosmas Prassides, University of Durham (UDUR), Durham, Great Britain Prof. Denis Arčon

- Combining Innovative Portable Visual, Accoustic, Magnetic and NMR Methods with In-situ Chemical Diagnostic Tools for Effective Failure Assessment and Maintenance Strategy of Rail and Subway Systems DIAGNO-RAIL
  - 7. FP. 262207

EC; Georgios Papavassiliou, Institute of Materials Science, NCSR Demokritos, Aghia Paraskevi, Attiki, Greece

Prof. Janez Dolinšek

Underwater Coastal Sea Surveyor

UNCOSS

7. FP, 218148

- EC; Dominique Vilbois, Patrick Peras, ECA SA, Toulon, France Prof. Robert Blinc, Prof. Aleksander Zidanšek
- Development of Wear Resistant Coatings based on Complex Metallic Alloys for Functional Applications
- appliCMA

7. FP 214407

EC; Andreas Merstallinger, Aerospace & Advanced Composites GmbH, Wiener Neustadt, Austria

- Prof. Janez Dolinšek, Asst. Prof. Miha Čekada, Asst. Prof. Kristoffer Krnel, Asst. Prof. Srečo D. Škapin
- Hierarchical Assembly in Controllable Matrices 5 HIERARCHY
  - 7. FP, 215851, PITN-GA-2008-215851

EC; Paul Kouwer, Harry Rullmann, Radboud University Nijmegen, Faculty of Science, Nijmegen, The Netherlands

- Prof. Igor Muševič 6. ESNAM European Scientific Network for Artificial Muscles COST MP1003
- EC; COST Office, Brussels, Belgium
- Prof. Boštjan Zalar, Dr. Blaž Zupančič Network for Intermetallic Compounds as Catalysts for Steam Reforming of Methanol IMC-SRM
- COST
- EC; COST Office, Brussels, Belgium
- Prof. Janez Dolinšek
- 8. Designing Novel Materials for Nanodevices: From Theory to Practise (NanoTP) COST MP0901
  - EC; COST Office, Brussels, Belgium Dr. Polona Umek
- Optical Micro-manipulation by Nonlinear Photonics COST MP0604
  - EC; COST Office, Brussels, Belgium
- Prof. Igor Muševič 10. Structure and Mechanism of Cytoplasmic Dynein
- HFSP RGP0009/2008-C
- HFSPO International Human Frontier Science Program Organisation, Strasbourg, France; University of Leeds, IMSB FBS, Leeds, Great Britain Asst. Prof. Andrej Vilfan
- 11. Targeting AntimicroBial Activity via micro/Nano-structured surfaces for civil Applications
  - TABANA
  - MNT-ERA-NET II
  - Univerza v Mariboru, Maribor, Slovenia
- Prof. Janez Štrancar 12. Novel States of Matter Induced by Frustration in Quantum Magnets
  - PROTEUS
  - BI-FR/11-12-PROTEUS-008
  - Prof. Philippe Mendels, Laboratoire de Physique des Solides Universite Paris Sud, Orsay, France
  - Dr. Andrei Zorko
- 13. Supermolecular Organization of Polisaharides in Marine Gel Networks BI-HR/10-11-011
- Dr. Vesna Svetličić, Ruđer Bošković Institute, Zagreb, Croatia Prof. Janez Štrancar
- 14. Hydrogen Storage in Metal Hydrides and Nanomaterials BI-KR11-12-002 Dr. Hae Jin Kim, Korea Basic Science Institute, Daejeon, Korea
  - Asst. Prof. Tomaž Apih
- 15. Multidrug Resistance in Cancer and Membrane Domain Structures BI-PL/10-11-009

Dr. Rochala Wojceich, The University of Warsaw, Warsaw, Poland Prof. Janez Štrancar

- 16. Molecular Dynamics Studies in Chiral Nematic and Smectic Phases by Proton NMR BI-PT/10-11-011
  - Prof. Pedro Sebastiao, Cenro de Fisica da Meteria Condensada da Universidade de Lisboa, Lisbon, Portugal Asst. Prof. Tomaž Apih
- 17. Dielectric and Electocaloric Properties of Advanced Relaxor Polymer Films and Nanotubes
- BI-US/09-12-039
  - Prof. Zhang Qiming, Office of Sponsored Programs, The Pennsylvania State University, PA, USA
- Asst. Prof. Vid Bobnar
- Geometrically Frustrated Quantum Magnetism BI-US/09-12-040
- Dr. Johan van Tol, National High Magnetic Field Laboratory, Florida State University, FL, USA
- Dr. Andrej Zorko

# **R &D GRANTS AND CONTRACTS**

- 1. Patterns, Structural Self-assemly and Multiferroic States in Mixtures of Nanoparticles and Liquid Crystals Prof. Samo Kralj
- 2. Physicochemical Processes Involved in Formation of Radioactive Nanoaerosols Prof. Janja Vaupotič
- 3. Advanced Ferroelectric Polymeric and Inorganic Materials: Giant Electrocaloric Effect and Transport Properties
- Prof. Zdravko Kutnjak Hydrogen Storage in Zr-based Metallic Glasses 4.
- Prof. Janez Dolinšek
- New Methods for the Detection of N-14 Nuclear Quadrupole Resonance Asst. Prof. Tomaž Apih
- 6 Novel Ground States and Quantum Critical Points in Low-dimensional Quantum Spin Systems
- Dr. Andrej Zorko
- 7. Molecular Motors
- Asst. Prof. Andrej Vilfan
- 8. Superconductivity and magnetism in new iron-based superconductors Dr. Peter Jeglič
- 9 Three Dimensional Assembling of Colloidal Structures in Mesophases Prof. Slobodan Žumer
- 10. Hybrid Nanomaterials for Low-friction Polymer Composites and Energy Conversion Prof. Maja Remškar
- 11. Optical Microresonators Based on Liquid Crystals Prof. Igor Muševič
- 12. New metallic materials for thermal storage of digital information
- Dr. Andraž Kocjan 13. Design, formulation and characterization of biomimetic nanocomposite systems for effective tissue regeneration
- Dr. Mojca Urška Mikac 14. Theory of the nematic nanodroplet and ordering of DNA, encapsidated in simple viruses
- Asst. Prof. Andrej Vilfan
- 15. Collective and molecular dynamics of photosensitive liquid crystal elastomers Prof. Martin Čopič
- 16. Use of Nanoparticles as Additives in Lubricants and in Tribology Prof. Maja Remškar
- 17. Textured Ceramic Films for Sensors and Actuators Prof. Marija Kosec
- 18. Use of green energy sources: New functional nanomaterials on the base of polyoxometalates and TiO2 nanostrucutres for production of hydrogen by catalytic oxidation of water -NANOleaf Dr. Polona Umek
- 19. Study of the structure and the dynamics of blood clot dissolution: mathematical modeling supported by magnetic resonance experiments Prof. Igor Serša
- 20. Dentin Evolution Detected by Spectroscopic Means
- Prof. Janez Štrancar 21. Study of Food Processing and Preparation by Magnetic Resonance Imaging and Spectroscopy Methods
- Prof. Igor Serša 22. Formulation and Characterization of BF Fuzogenic Nanoparticles for Efficient Drug Delivery into Cells Dr. Marjeta Šentjurc
- 23. Oligomers of amyloidogenic proteins from a to z: biophysical properties, structure,



function and mutual interactions

- Prof. Eva Žerovnik
- 24. Applications of Nanoparticle Macromolecule Complexes for the Formulation of **Biological Drugs**
- Prof. Igor Muševič Wireless Networks with Radio over Optical Fiber 25
- Prof. Jurij Franc Tasič
- 26. Behaviour of disipative systems under extreme termo-mechanical loading Dr. Matej Pregelj
- New materials for power conversion: Oxide semiconductor thermoelectrics 27 Prof. Danilo Suvorov
- Biotechnological Processes of Treatment of Lignocellulosic Materials 28. Prof. Janez Štrancar
- Eye Protection Dr. Janez Pirš
- A spectrometer for automatic 14N nuclear quadrupole resonance characterization of 30. new substances Dr. Alan Gregorovič

## **MENTORING**

#### Ph. D. Theses

- 1. Biljana Govedarica, Evaluation of mechanical and surface properties of pharmaceutical materials and products on a single particle level by atomic force microscopy (mentor Stane Srčič: co-mentor Miha Škarabot).
- Stane Pajk, Influence of some cholesterol oxidation products on the structure of model 2 membranes (mentor Slavko Pečar; co-mentor Janez Štrancar).
- Igor Perkon, Analysis of whisker dynamics by tracking of non rigid open curves 3. (mentor Jurii F. Tasič: co-mentor Mathew Diamond).
- Mojca Rangus, The study of structural characteristics and formation of microporous 4 and mesoporous materials (mentor Gregor Mali; co-mentor Janez Seliger).

#### M. Sc. Thesis

1. Sweety Karta Ram, Sustainable agriculture in India : need and prospects with particular reference to the state of Punjab (mentors Ivo Šlaus, Peter Stanovnik, Matej Stopar, Gojmir Lahajnar).

# VISITORS FROM ABROAD

- Dr. Mirta Herak, Institute of physics, Zagreb, Croatia, 1. 1. 2011 31. 12. 2011. 1.
- Prof. Dr. Shiro Kashimoto, Hokkaido University, Faculty of Engineering, Division of 2. Applied Physics, Sapporo, Hokkaido, Japan, 1. 1. 2011 - 30. 9. 2011.
- Hyun Wook Kang in Go Woon Lee, Korea Basic Science Institute, Daejeon, South Korea, 3. 3. 1. 2011 - 4. 3. 2011.
- Dr. Marija Raguž, School of medicine, Department of Medical Physics and Biophysics, 4 Split, Croatia, 25. 1. 2011 - 26. 1. 2011.
- 5. Dr. Oksana Zaharko, ETHZ & Paul Scherrer Institute, Laboratory for neutron scattering, Villingen, Switzerland, 27. 1. 2011 - 29. 1. 2011.
- Prof. Dr. Pedro Sebastiao in prof. dr. Maria Helena Godinho, Instituto Superior Tecnico, 6 Department of physics, Lizbon, Portugal, 30. 1. 2011 - 6. 2. 2011.
- 7. Mantas Šimenas, University of Villniusu, Faculty of Physics, Villnius, Lithuania, 1.2 2011 - 20. 7. 2011.
- Evangelia Karatairi, NCSR Demokritos, Aghia Paraskevi, Greece, 4. 2. 2011 6. 2. 2011. 8 Dr. Valentina Domenici, Department of Chemistry and Industrial Chemistry, University 9
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- 10. Dr. Marco Bonora, University of Pavia, Pavia, Italy, 17. 3. 2011 18. 3. 2011.

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- Asst. Prof. Tomaž Apih 1.
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- Asst. Prof. Vid Bobnar 4
- Asst. Prof. Pavel Cevc, retired 28.12.11 5. Prof. Janez Dolinšek\*
- 6.
- 7. Dr. Cene Filipič 8. Dr. Peter Jeglič

- RESEARCH PROGRAMS
- 1 NMR and Dielectric Spectroscopy Condensed Matter Prof. Janez Dolinšek
- 2. Physics of Soft Matter, Surfaces and Nanostructures Prof. Slobodan Žumer
- 3. Experimental Biophysics of Complex Systems Prof. Janez Štrancar

### NEW CONTRACT

- 1. Development of technologies for artificial nose Ministry of Defence Prof. Igor Muševič
- 11. Prof. Dr. Horst Beige, University of Martin-Luther, Halle, Germany, 21. 3. 2011 24. 3. 2011.
- Dr. Jong-Hwa Kim, Korea Basic Science Institute, Analysis Research Division, Daegu Center, Daegu, South Korea, 15. 3. 2011 - 31. 12. 2011
- Prof. Dr. Arcady Levanyuk, Department of Condensed Matter Physics, Faculty of 13. Science, Cantoblanco Campus, Madrid, Spain, 10. 4. 2011 - 10. 5. 2011.
- 14. Dr. Darija Jurašin, Institute of Ruđer Bošković, Zagreb, Croatia, 31. 5. 2011 30. 11. 2011. Dr. Magdalena Wencka, Institute of Molecular Physics, Polish Academy of Sciences, 15.
- Poznan, Poland, 1. 5. 2011 31. 5. 2011, 1. 10. 2011 31. 10. 2011. 16. Surajit Dharo, University of Hyderabad, School of Physics, Hyderabad, Andhra Pradesh, India, 1. 5. 2011 - 3. 6. 2011.
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- 21 Dr. Vassilios Tzitzios, NCSR Demokritos, Aghia Paraskevi, Greece, 1. 6. 2011 - 26. 7. 2011. Prof. Dr. Sergio Diez Berart, Technical University of Catalonia, Department of Physics 22.
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- 25 Dr. Fabrice Bert, Universite Paris Sud 11, Laboratory of Solid State Physics, Paris, France, 19. 7. 2011 - 22. 7. 2011.
- Dr. Tihomir Betti, University of Split, Faculty of Electrical Engineering, Mechanical 26. Engineering and Naval Architecture, Split, Croatia, 15. 8. 2011 - 31. 8. 2011.
- Doc. Dr. Denis Stanić, University of Osijek, Osijek, Croatia, 1. 9. 2011 30. 9. 2011.
- Dr. Wolfgang Porod, University of Notre Dame, Department of Electrical Engineering, Indiana, USA, 19. 9. 2011 - 22. 9. 2011.
- Dr. Michael Averbukh, Ben Gurion University, Beer Sheva, Israel, 1. 9. 2011 30. 9. 2011. 29. Prof. Dr. Kalpathy Easwaran, Indian Institute of Technology, Bangalore, India, 3. 9.
- 2011 6. 9. 2011. Prof. Dr. Tim Sljuckin, Southampton University, Southampton, United Kingdom, 1. 10. 2011 - 30. 12. 2011.
- 32. Dr. Sebastian Turczynski, Institute of Electronic Materials Technology, Warsaw, Poland, 20. 10. 2011 - 20. 11. 2011.
- Fabian Vaca Chavez, Instituto Superior Tecnico, Lisbon, Portugal, 20. 11. 2011 26. 11. 2011. 33
- 34. Dr. Lia Verhoeff, Utrecht University, Van't Hoff Laboratory for Physical and Colloid Chemistry Debye Institute, Utrecht, Netherlands, 26. 11. 2011 - 17. 12. 2011.

- 10. Prof. Samo Krali\*
- 11. Prof. Zdravko Kutnjak
- 12. Prof. Gojmir Lahajnar, retired 31.12.11
- 13. Prof. Adrijan Levstik
- 14. Dr. Mojca Urška Mikac 15. Prof. Igor Muševič\*, Head
- 16. Dr. Andriy Nych, left 27.09.11
- 17. Prof. Slavko Pečar\*, retired 01.11.11

- 18. Dr. Janez Pirš 19. Asst. Prof. Dušan Ponikvar\* 20. Prof. Albert Prodan 21. Prof. Maja Remškar 22. Prof. Janez Seliger\* 23. Prof. Igor Serša 24. Prof. Janez Stepišnik 25. Asst. Prof. Miha Škarabot 26. Prof. Janez Štrancar 27. Prof. Jurij Franc Tasič\* 28. Dr. Polona Umek 29. Dr. Herman Josef Petrus Van Midden 30. Asst. Prof. Andrej Vilfan 31. Prof. Boštjan Zalar 32. Prof. Aleksander Zidanšek 33. Dr. Andrej Zorko 34. Prof. Slobodan Žumer\* Postdoctorial associates 35. Asst. Prof. Zoran Arsov 36. Daniele Biglino, B. Sc. 37. Dr. Alan Gregorovič 38. Dr. Tilen Koklič 39. Dr. Uliana Ognysta, left 27.09.11 40. Dr. Matej Pregelj 41. Dr. Uroš Tkalec 42. Dr. Jernej Vidmar\* 43. Dr. Stanislav Vrtnik 44. Dr. Blaž Zupančič 45. Dr. Erik Zupanič Postgraduates 46. Franci Bajd, B. Sc. 47. Nina Bizjak, B. Sc.
   48. Matej Bobnar, B. Sc. 49. Goran Casar, B. Sc. 50. Ana Dergan, B. Sc. 51. Andreja Eršte, B. Sc. 52. Maja Garvas, B. Sc. 53. Anton Gradišek, B. Sc. 54. Matjaž Humar, B. Sc. 55. Ivan Iskra, B. Sc. 56. Venkata Subba Rao Jampani, M. Sc. 57. Simon Jazbec, B. Sc.
- 58. Andreja Jelen, B. Sc.

# BIBLIOGRAPHY

#### ORIGINAL ARTICLES

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# 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 together 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 nano-electronics. These and other materials, such as strongly correlated systems, electronically ordered systems and superconductors were investigated using Head: advanced femtosecond spectroscopy techniques. In many areas we have introduced new materials, technologies Prof. Dragan D. Mihailović and techniques.



#### Ultrafast studies of electron dynamics in correlated systems.

The field of the 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 on-going 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 makes it

#### We observed remarkable anharmonic effects, hitherto undetected in the systems exhibiting collective charge ordering.

possible to distinguish different components by their lifetimes. Moreover, the relaxation kinetics can yield valuable information about the mechanism for superconductivity.

By means of the three-pulse method we also investigated the excitation region below the CDW destruction threshold in 17-TaS2 and TbTe3. Upon strong coherent excitation we observed self-modulation of the amplitude mode intensity. A similar effect was also observed for some other phonons, where the cross-modulation at the amplitude-mode frequency indicates the anharmonic interaction of those phonons with the amplitude mode. By analysing the observed phenomena in the framework of time-dependent Ginzburg-Landau theory we attribute the effects to the anharmonicity of the mode potentials inherent to the broken symmetry state of the CDW systems. The results were published in Phys. Rev. B 83, 035104 (2011).

We investigate the relaxation dynamics of photo-excited quasiparticles (QPs) in underdoped Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+8</sub>  $(T_{e}=78 \text{ K})$ . By changing the excitation energy and polarization of the probe beam, two different types of relaxation

dynamics, associated with superconducting (SC) and pseudo-gap (PG) QPs, are quantitatively analysed independently. The pump fluence (F) dependence of the SC-dominated transients shows a contribution of the PG component above the saturation condition of the SC component where Cooper pairs with long-range order are fully destroyed within the photo-excited volume. Assuming a temperature-independent PG decay time, we successfully isolate the native SC transient even above the threshold by subtracting the PG response from the original data. In the saturation regime, the exponential decay (recovery of SC) is fast (2-3 ps), suggesting an efficient non-equilibrium phonon relaxation in this compound. We also find a flat-top response preceding the exponential decay above the threshold, which appears as a

delay of the SC recovery in the original data. This response is visible over



Figure 1: Tracking the melting of charge density waves using a femtosecond electron-diffraction camera.

the whole temperature range below T<sub>e</sub> and its duration increases with increasing F. The response is attributable to a photo-induced SC-to-non-SC phase transition arising from an excitation by the non-thermal QPs and/or high-frequency phonons. The consistently near-constant magnitude of the PG response at the start of the SC state recovery from the non-SC phase suggests a correlation between the SC and PG QPs. The results were published in Phys. Rev. B84, 174516 (2011).

The processes leading to non-thermal condensate vaporization and charge-density-wave (CDW) melting with femtosecond laser pulses is systematically investigated in different materials. We find that vaporization is relatively slow ( $\sim$ 1 ps) and inefficient in superconductors, exhibiting a strong systematic dependence of the vaporization energy on the critical temperature. In contrast, melting of the CDW order proceeds rapidly (50–200 fs) and more efficiently. A quantitative model describing the observed systematic behaviour in superconductors is proposed based on a phonon-mediated quasiparticle (QP) bottleneck mechanism. In contrast, Fermi-surface disruption by hot QPs is proposed to be responsible for the CDW state melting. The results were published in Phys. Rev. B 84, 180507 (2011).

The transient photo-induced reflectivity and the transient photo-induced magneto-optical Kerr angle were measured in a  $La_{0.875}Sr_{0.125}MnO_3$  single crystal as functions of temperature. A separate photo-induced transient ferromagnetic phase is found to form within the pseudo-cubic low-temperature insulating ferromagnetic phase after photo-excitation. The characteristic time of the transient phase formation is of the order of 10 ps. The similarity with  $Pr_{0.6}Ca_{0.4}MnO_3$  indicates that the photo-induced transient ferromagnetic phase is a general property of the insulating ferromagnetic state in colossal-magnetoresistive manganites. The results were published in **Phys. Rev. B 83, 113103 (2011)**.

The dynamics for both salts show similar temperature dependences, which is well characterized by the carrier relaxation across the pseudo-gap (PG) of the magnitude  $\Delta PG \approx 16$  meV for Br salt and 7.0 meV for Cl salt. On the

We investigated the relaxation dynamics of non-equilibrium carriers in organic conductors κ-(BEDT-TTF)2Cu[N(CN)2]X (X=Br and Cl) using ultrafast time-resolved optical spectroscopy. other hand, only the Br salt shows an abrupt increase of the decay time at low temperature, indicating an additional decay component associated with the superconducting (SC) gap below the Tc. The fluence-dependent dynamics at low temperature evidence the superposition of the SC component onto the PG component. These results indicate a metallic-insulating phase

separation in the Br salt triggered by photo-excited non-equilibrium carriers. The results were published in Phys. Rev. Lett. 107, 227002 (2011).

We also extended systematic investigations of the electron phonon coupling into several cuprate and ironbased pnictide superconductors and charge density wave compounds. The manuscript reporting these results is currently in preparation.

We continued our research of the relaxation of quasiparticles in pnictide superconductors. We systematically investigate the photo-excited (PE) quasi-particle (QP) relaxation and low-energy electronic structure in electron doped Ba(Fe<sub>1x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> single crystals as a function of Co doping. The evolution of the photo-induced reflectivity



Figure 2: Energy required to vaporize the superconducting condensate Uv, expressed in K per planar Cu as a function of Tc2 for cuprates. The data for NbN, SmFeAs<sub>00.5</sub>F<sub>0.2</sub> and  $a(Fe_{0.93} Co_{0.07})_{a}As_{2}$  are included for comparison. The solid line is a plot of Ulost where Uv=Uc+Ulost (Uc is condensation energy).

Dashed line is a square law  $Uv=\eta Tc2$ , where  $\eta=1.5\times 10^3 K^2$  atom<sup>1</sup>. The inset shows the phonons with  $h\infty>2\Delta$  which can break the pairs. The measured phonon density of states for YBCO is approximated by a parabola. transients with x proceeds with no abrupt changes. In the orthorhombic spin-density-wave (SDW) state a bottleneck associated with a partial charge-gap opening is detected, similar to previous results in different SDW iron-pnictides. The relative charge gap magnitude decreases with increasing x. 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 behaviour the optical SC-state destruction energy is determined near the optimal doping. The subsequent relatively slow recovery of the SC state indicates clean SC gaps. The T-dependence of the transient reflectivity amplitude in the normal state is consistent with the presence of a pseudo-gap in the QP density of states. The polarization anisotropy of the transients suggests that the pseudo-gap-like behaviour might be associated with a broken point symmetry resulting from nematic electronic fluctuations persisting up to  $\sim 200$ K at any x. The second moment of the Eliashberg function, obtained from the relaxation rate in the metallic state at higher temperatures, indicates a moderate electron phonon coupling,  $\sim 0.3$ , that decreases with increasing doping. The manuscript was submitted to Physical Review.

#### Theoretical studies on the nanoscale

Unconventional symmetries of the order parameter allowed some researchers to maintain that a purely repulsive interaction between electrons provides superconductivity without phonons in a number of high-temperature superconductors. We have analysed the problem of unconventional superconductivity with the repulsive interaction and have shown that the Cooper pairing with small orbital moments is strongly suppressed by the realistic Coulomb repulsion between fermions at relevant temperatures in any dimension (Physical Review Letters, 106, 136403 (2011)).

Our results show that these bifurcations can substantially complicate the dynamics of the order parameter and eventually lead to the appearance of such phenomena as multi-stability and chaos. The discussed bifurcation phenomena shed a light on some recent experimental findings (Physical Review B, 84, 094527 (2011)). The current-voltage characteristics of long and narrow superconducting channels are investigated using the time-dependent Ginzburg-Landau equations for the complex order parameter. We found that the steps in the current-voltage characteristic can be associated with bifurcations of either a steady-state or oscillatory solution.

#### Nanomaterials

Inorganic molecular wires – particularly molybdenum halide or chalcogenide cluster polymers – have emerged as a new type of one-dimensional materials with remarkable molecular-scale functionality. Their one-dimensional polymer structure gives rise to some very unusual physical properties. Anionic bridges which bind Mo clusters together into one-dimensional chains are extraordinarily strong, yet highly deformable, giving rise to exception-ally 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 easy dispersion in common polar solvents and ultra-low shear moduli, on the other. The sulphur atoms within the structure facilitate diverse functionalization chemistry to thiol-containing molecules, such as proteins.

We have demonstrated the use of a novel electrochemical sensing platform based on aptamer conjugated  $Mo_6S_9$ ,  $x_1x$  nanowires (MoSI NWs) for the highly sensitive detection of the blood-clotting enzyme thrombin. MoSI NWs were self-assembled on a gold electrode to which thrombin binding aptamers were covalently attached. The modification and immobilization steps of the electrodes were characterised by cyclic voltammetry along with high-resolution transmission electron microscopy and X-ray photoelectron spectroscopy. The platform was based on the creation of a self-assembled MoSI NW layer via the sulphur-gold affinity followed by the creation of MoSI-thiolated aptamer

conjugates via the sulphur-sulphur affinity. Using this system, the sensitive quantitative detection of thrombin was realized by monitoring the differences of the differential pulse voltammetric responses of electrostatically trapped [Ru(NH<sub>3</sub>)<sub>6</sub>]<sup>3+</sup> cations to the aptamer before and after thrombin binding. Given the direct label-free nature of the approach and the simplicity of the electronic detection, the aptamer conjugated MoSI NWs biosensor appears

well suited for implementation in portable point of care microdevices directed at the rapid and sensitive detection of proteins and pathogens. These results are reported in **Biosensors & Bioelectronics**, 26, 1853-1859 (2011).

We have determined the work function W of  $Mo_6S_3I_6$  molecular nanowires using Kelvin probe (KP) measurements, UV photoelectron spectroscopy (UPS), and cyclic voltammetry (CV). The values obtained by all three methods agree well, giving the value W = 4.8 + /-0.1 eV. CV measurements also indicated a gap between the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of Eg = 1.2 + /-0.1 eV, in agreement with recent optical measurements, but in disagreement with theoretical calculations, which have predicted the materials to be metals. The electronic structure of  $Mo_6S_3I_6$  suggests the use of the material in applications such as bulk heterostructure photovoltaics and transparent electrodes and for molecular electronics devices. This work was presented in Langmuir, 27, 4296-4299 (2011).

#### Electron dynamics in biological macromolecules

Firstly, we have determined the optimal concentration conditions for the M-DNA complex formation, trying to avoid an unwanted aggregation of DNA, which could happen in the presence of an overcritical concentration

of divalent cations. In the next step we were looking for the most reliable methods for the deposition, stretching and aligning of long ( $\sim 10\,\mu m$ ) DNA molecules on appropriate substrates (Si/SiO<sub>2</sub> wafers, mica). We found that by slow (3 cm/min) extraction of the substrate from a DNA solution with a computer-controlled step motor we could obtain stretched, long, DNA double helices on the surface of the substrate. The final step in the sample

preparation for electronic transport measurements on individual M-DNA macromolecules is the positioning of the macromolecules on or between micron- or submicron-sized electrical contacts. By the positioning of the individual M-DNA molecules between the electrical contacts at distances of  $\sim 1 \,\mu$ m for two-probe measurements of electrical conductivity we could achieve a method of dielectrophoresis. This method requires a determination of the optimal values for the relevant parameters – frequency and amplitude of an AC electrical field, DNA and ion concentrations

The sensitivity limit for the detection of thrombin was 10 pM. This value is 10-fold better than all the currently reported one-step, label-free electrochemical strategies.

In 2011 we started to develop methods for electronic transport measurements on individual

macromolecules of DNA complexes with

transition-metal cations, i.e., M-DNA.

and the duration of each dilectrophoresis run. In a relatively short time we have succeeded in determining the optimal dielectrophoresis parameters for our system and now we are able to position individual M-DNA molecules

In 2011 we continued with investigations of optical holographic patterning in light-sensitive liquid-crystal elastomers (LCEs).

or bundles of them in the submicron spaces between electrical contacts with great reproducibility. The development of a method for the deposition of stretched M-DNA molecules on a grid of four or more electrodes is currently in progress. The method will be based on forcing a flux of DNA solution through a microfluidic channel which will be mounted directly over the

electrodes. Such prepared samples will enable us to conduct four-probe measurements of the electric conductivity and to manufacture simple electronic devices, which is indeed the final goal of our research on M-DNA complexes as building blocks in molecular nanoelectronics.

#### Soft Matter

These are polymer materials that exhibit a very strong opto-mechanical response, due to which they are promising for applications in various optically manipulated micromechanical devices. An important factor for the optical



Figure 3: Characterization of optical diffraction grating in light-sensitive liquid-crystal elastomer – angular dependence of diffracted intensity in the vicinity of the Bragg peak for different recording times: (a) experiment, (b) theoretical prediction.

manipulation is the absorption depth of the material. In relation to this we investigated the unusual phenomenon of a strong increase in the depth of recorded holographic patterns with recording time. We showed that this effect is related to a decrease of the absorption coefficient due to the photo-isomerization process. The results are reported in the paper Phys. Rev. E 84, 031707-1-5 (2011).

We restarted our 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 found that the addition of only 0.1 wt% of MoSI nanowires to the commercial liquid-crystal mixture (TL203, Merck) causes a significant reduction of the switching voltage and a profound increase of the switching speed. These findings suggest that the doping of liquid crystals with suitable nanoparticles is one of the promising strategies for further improvements in the technology of liquid-crystal displays (LCDs) and other optical devices based on liquid crystals. The results are described in the paper **Sensors & Transducers Journal 12, 18-25 (2011)**.

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. The main goal of these investigations is the fabrication of a new type of polarizers and analysers for cold neutrons. The preliminary results are reported in the paper, which is accepted for publication in J. Phys.: Conference Series.

Our investigations of the self-assembling properties of DNA-related molecules were in 2011 focused onto two problems: (i) 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) a comparative study of the aggregation properties of four very similar G-rich DNA oligonucleotides in an aqueous solution. The investigations of the latter showed that all four oligonucleotides formed G-quadruplex structures. However, in contrast to the expectations from some other experiments, our results suggest that the formation of tertiary structures (G4-wires) is less profound in the derivatives containing the so-called "sticky CG ends" than in the derivative without the GC ends.

Using dynamic light scattering we studied the temperature dependence of the scattered intensities and relaxation rates for pure twist and pure bend modes in a colloidal system of  $BaTiO_3$  single-domain ferroelectric nanoparticles and liquid crystal 8CB close to the nematic-to-smectic A phase transition. From the experiments we obtained the critical exponents for the smectic correlation lengths, which in suspensions differ from the values for the pure 8CB and are close to the predicted values of the mean field theory. The phase-transition temperatures from the isotropic to nematic phase  $T_{_{NI}}$  and from nematic to smectic A phase  $T_{_{NA}}$  are both affected by the presence of the particles in two ways. The electric field around the ferroelectric particles increases the

#### Different methods for the holographic patterning of composite materials made from photopolymer and superparamagnetic nanoparticles were analysed.

transition temperatures, while the disorder and probably also the excess of the surfactant cause a decrease of the transition temperatures compared to pure 8CB. Both effects result in lower  $T_{_{NI}}$  and almost unchanged  $T_{_{NA}}$  in suspensions. After prolonged exposure to the external field the ferroelectric particles irreversibly aggregate, which results in a decrease of the internal electric field and, consequently, in a decrease of both transition temperatures.

Using passive micro-rheology we measured the micro-rheological properties of a magnetic fluid as a function of the direction and magnitude of the external magnetic field. The effective microviscosity strongly depends on the

magnitude of the external field, while it is almost independent of its direction. It vanishes in zero field, while in nonzero field it is larger by a factor of 2 to 4 in the direction along the field than perpendicular to it. The non-zero value of the storage modulus, which indicates the formation of a viscoelastic fluid, appears at magnetic fields at which the dynamic light scattering experiments reveal the formation of elongated structures. The results are reported in **Soft Matter**, **7**, **125-131 (2011)**.

#### 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 the National Institute for Materials Science in Tsukuba, Japan, (LiTaO3) and North Carolina State University in Raleigh, USA, (GaAlN) we study new concepts of compact light sources on the basis of the nonlinear optical conversion of existing lasers into the spectral regions where lasers are not yet available. In cooperation with Rainbow Photonics A.G., a spin-off company of ETH Zurich, we collaborate on 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. It will operate at a fixed frequency difference of 9.3 THz.

The main part of the work was devoted to an investigation of the different types of lensing effects in Ruby and Nd:YAG lasers. The obtained results are reported in the paper **Applied Physics B 105**, 793-800 (2011).

#### **Biomedical optics**

Using such PPTR profiling and a dedicated numerical model, we have developed a unique method for a determination of the maximum safe laser radiant exposure of human skin. The current, purely subjective, approach to a determination of this value for each patient and treatment site, namely, significantly affects the efficacy and safety of many dermatologic laser treatments. We have demonstrated that our technique provides more accurate and reliable values than earlier attempts using the same clinical input.

Using our laboratory PPTR setup, we have measured laser-induced temperature profiles over the course of the removal of unwanted tattoos in human volunteers (in collaboration with Fotona d.d., Ljubljana). Our

technique has shown a unique potential for the characterization of pulsed-laser interaction with tattooed skin, objective monitoring of therapeutic efficacy, and adjustment of the treatment on an individual patient basis. For

future clinical trials, we have developed a portable PPTR profiling device and tested its performance using laboratory tissue models.

We have upgraded a Monte Carlo model of optical transport in skin with a novel approach to the treatment of the volume of interest's side boundaries. Our approach allows high-resolution modelling of skin inclusions with complex geometries and arbitrary irradiation patterns at significantly lower computational demands as compared to earlier documented methods. Using this model, we have performed a parametric study of blood vessel photocoagulation and collateral tissue damage in a novel treatment of port-wine stain (PWS) lesions using sequential laser irradiation and intermittent cryogen spray cooling (collaboration with Beckman Laser Institute and Medical Clinic, University of California at Irvine).



Figure 4: Traces and corresponding mean square displacements of a probe particle show highly anisotropic micro-rheological properties of magnetic colloid in external magnetic field.

The measured effective storage modulus in magnetic colloid varies significantly within the sample and depends on both the direction and the magnitude of the external magnetic field.



Figure 5: BAM (Brewster-angle microscopy) image of heptadecanoic acid film at the air/water interface.

ad adjustment of the treatment on an individual patient basis. For le PPTR profiling device and

- In cooperation with the laser company Fotona d.d. from Ljubljana we continued with the development of computer-simulation methods for a determination of the optical field in unstable laser resonators.
- We have investigated the potential of pulsed photo-thermal radiometry (PPTR) for noncontact measurements of laser-induced temperature profiles in strongly scattering biological tissues.

#### **Biological systems**

In collaboration with the *Laboratory for Experimental Soft Matter* at *Faculty of Mathematics and Physics, University of Ljubljana*, we continued research of biomimetic systems with an emphasis on artificial cilia.

We used magneto-optical tweezers to assemble micrometre-sized superparamagnetic spheres into long chains that were attached to a glass surface on one end. This created an array of artificial cilia and we investigated the



Figure 6: Magnetically driven artificial cilia mimic the motion of biological cilia.

By using an external magnetic field, we rotated the cilia and the asymmetry of rotation resulted in a fluid flow. hydrodynamics around them. We focused on the research of hydrodynamic coupling between individual cilia, which presumably leads to the generation of metachronal waves on a cell surface. Such waves more efficiently pump the liquid or propel a swimming unicellular microorganism. Our findings were published in **Biomicrofluidics 5**, 034103 (2011).

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. Using the model we found the most efficient beating pattern both of a single cilium and of a densely ciliated surface, where metachronal coordination was shown to have a strong effect on the pumping efficiency. We proved that microorganisms swim with high energetic efficiency, which is contrary to previous beliefs. The work was published in **Proceedings of National Academy of Sciences (PNAS)**, 108, 15727 (2011).

#### Some outstanding publications in 2011

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#### Some outstanding publications in 2009

- 1. Strle, Jure, Vengust, Damjan, Mihailović, Dragan. Inorganic molecular-scale MoSI nanowire-gold nanoparticle networks exhibit self-organized critical self-assembly. Nano lett. (Print), 2009, vol. 9, no. 3, str. 1091-1095.
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- Mertelj, Tomaž, Kabanov, Viktor V., Gadermaier, Christoph, Zhigadlo, N. D., Katrych, S., Karpinski, J., Mihailović, Dragan. Distinct pseudogap and quasiparticle relaxation dynamics in the superconducting state of nearly optimally doped SmFeAsO[sub](0.8)F[sub](0.2) single crystals. Phys. rev. lett., 2009, vol. 102, no. 11, str. 117002-1-117002-4.
- 5. Petelin, Andrej, Čopič, Martin. Observation of a soft mode of elastic instability in liquid crystal elastomers. Phys. rev. lett., 2009, vol. 103, no. 7, str. 077801-1-077801-4.
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#### Patents granted

- Process for the synthesis of nanotubes and fullerene-like nanostructures of transition metal dichalcogenides, quasi one-dimensional structures of transition metals and oxides of transition metals Aleš Mrzel, Maja Remškar, Adolf Jesih, Marko Viršek US8007756 (B2), United States Patent and Trademark Office, 30.8.2011.
- Multistable liquid crystal device Theo Rasing, Sergiy Lazarenko, Igor Muševič, Miha Škarabot, Marko Uplaznik EP1927885 (B1), European Patent Office, 27.7.2011.
- Laser system for medical and cosmetic applications Karolj Nemes, Matjaž Lukač EP2030586 (B1), European Patent Office, 11.5.2011.
- Laser system for medical removal of body tissue Matjaž Lukač, Marko Marinček, Marko Kazič, Karolj Nemes
  - US7867224 (B2), United States Patent and Trademark Office, 11.1.2011.
- Method for operating a laser system for bleaching teeth Matjaž Lukač, Boris Cenčič US8011923 (B2), United States Patent and Trademark Office, 6.9.2011.

#### Organization of conferences, congress and meetings

1. SLONANO 2011, Ljubljana, Slovenia, co-organizers, 26–28 October 2011.

# INTERNATIONAL PROJECTS

- 1. Next Generation Hybrid Interfaces for Spintronic Applications HINTS
  - 7. FP, 263104
  - EC; CNR, Consiglio Nazionale delle Ricerche, Rome, Italy Prof. Viktor Kabanov
- 2. Electronic Response of Single Inorganic Nanowires ERESIN
  - 7. FP, 230975, PERG03-GA-2008-230975a EC
  - Prof. Dragan Mihailović
- 3. Composites of Inorganic Nanotubes and Polymers COINAPO
- COST MP0902
- 4. EC; COST Office, Brussels, Belgium
- Prof. Dragan Mihailović
- Self-assembled Guanosine Structures for Molecular Electronic Devices COST MP0802 COST-Workshop-MP0802-01830 CCA M0802 1
  - CGA-MP0802-1
  - EC; Dr. Caroline Whelan, Kent Hung, COST Office, Brussels, Belgium Prof. Martin Čopič, Asst. Prof. Lea Spindler
- Electron-phonon Coupling in High-Temperature Superconductors Determined from Femtosecond Electron Relaxation Rates
  - BI-IT/11-13-001
  - Prof. Giulio Cerullo, ULTRAS-INFM-CNR, Dipartmento di Fisica Politecnico di Milano, Milano, Italy
  - Prof. Viktor Kabanov
- 7. Photonic Structures Based on Polymer-nanoparticle Composites BI-CN/11-13-012

Prof. Xinzheng Zhang, Ultrafast Photonics Lab. Teda Applied Physics School, Nankai University, Tianjin, China Prof. Irena Drevenšek Olenik

- Time Resolved Optical Spectroscopy of Collective Electronically Ordered States in Iron Based Pnictides
- BI-CN/11-13-003

Prof. Zhuan Xu, Department of Physics, Zhejiang University, Hang Zhou, China Prof. Viktor Kabanov

 Crystal and Film Growth and Time-domain Optical Spectroscopy Investigations of the Supeconducting State of the Cuprate Superconductors BI-CN/11-13-014

Prof. Xin Yao, Department of Physics, Shanghai Jiao Tong University, Shanghai, China Asst. Prof. Tomaž Mertelj

- Light-Sensitive Nanocomposite Media for Tunable Photonic Devices BI-CN/09-11-016
  - Prof. Xinzheng Zhang, Teda Applied Physics School, Nankai University, Tianjin, China Prof. Irena Drevenšek Olenik
- Age Determination of Traumatic Bruises by Combined Diffuse Reflectance Spectroscopy and Pulsed Photothermal Radiometry BI-NO/11-12-015

Asst. Prof. Lise Lyngsnes Randeberg, Norwegian University of Science and Technology, Department of Electronics and Telecommunications, Trondheim, Norway Prof. Boris Majaron

 Experimental Search for Collective Excitations in the Peierls Conductors by Optical Methods BI-RU/10-11-003

Dr. Sergei Zaitsev-Zotov, Kotelnikov Institute of Radioengineering and Electronics of

# MENTORING

#### Ph. D. Theses

- 1. Miha Devetak, Self-assembly of guanosine derivates on surfaces (mentor Irena Drevenšek Olenik).
- Martin Gorjan, Mid-infrared erbium doped fiber laser (mentor Martin Čopič; co-mentor Marko Marinček).
- Mathieu Lu-Dac, Phase slip phenomena and vortex dynamics in mesoscopic superconductors (mentor Viktor V. Kabanov).
- Jure Strle, Self-assembled MoSI nanowire networks and their properties (mentor Dragan Mihailović).

RAS, Moscow, Russia

- Prof. Viktor Kabanov
- Ultrafast Pump-probe Spectroscopy of Complex Matter e-GAP
  - Royal Society International Joint Projects 2009/R2
  - Prof. Sasha Alexandrov, Loughborough University, Physics Department, Loughborough, Great Britain
  - Prof. Dragan Mihailović
- 14. Laser Therapy of Cutaneous Vascular Lesions using Repetitive Irradiation and Intermittent
  - Cryogen Cooling BI-US/09-12-044

DFUS(V9)12-044 Dr. John Stuart Nelson, Beckman Laser Institute and Medical Clinic, University of California at Irvine, Irvine, USA

- Prof. Boris Majaron
  15. Laser Therapy of Cutaneous Vascular Lesions using Repetitive Irradiation and Intermittent Cryogen Cooling
  BI-US/09-12-044
  Dr. John Stuart Nelson, Beckman Laser Institute and Medical Clinic, University of
  - California at Irvine, Irvine CA, USA Asst. Prof. Boris Majaron 5. Structure and Dynamics of Confined Bent-core Liquid Crystals
- Structure and Dynamics of Confined Bent-core Elquid Crystals BI-US/08-10-029
   Noel A. Clark, Department of Physics, University of Colorado, CO, USA Prof. Martin Copič

# R &D GRANTS AND CONTRACTS

- 1. Dynamics of Complex Functional States
- Prof. Dragan Dragoljub Mihailović
  Sinthesis and characterization of novel nanostructures on the basis of transition metal Dr. Aleš Mrzel
- Molecular elecronics with MoSI nanowires Prof. Dragan Dragoljub Mihailović
- Biomimetic sistems in microfluidic
- Dr. Mojca Vilfan
- 5. Molecular Motors
- Asst. Prof. Andrej Vilfan 6. Ultrafast electron dynamics in metals and determination of electron-phonon coupling constant in metals and superconductors
- Prof. Viktor Kabanov 7. Cosmology in the lab - femtosecond control of phase transitions in real time Prof. Dragan Dragoljub Mihailović
- Collective and molecular dynamics of photosensitive liquid crystal elastomers Prof. Martin Čopič

### **RESEARCH PROGRAMS**

- 1. Light and Matter
- Prof. Martin Čopič
- 2. Dynamics of complex nano-systems Prof. Dragan Dragoljub Mihailović

#### M. Sc. Thesis

1. Luka Cmok, Dynamic light scattering in suspensions of ferroelectric nanoparticles in liquid crystals close to nematic to smetic A phase transition (mentor Alenka Mertelj).

### VISITORS FROM ABROAD

- dr Venera Nasretdinova, Kotel'nikov Istitute of Radioengineering and Electronics of RAS, Moscov, Rusia, 29–25 February 2011.
- Marina Davydova, Institute of Physics of the Academy of Sciences of the Czech Republic, Prague, Czech Republik, 1 February to 1 May 2011.

- 3. dr Gary Cook, Air Force Research Laborathory, Ohio, USA, 07-11 March 2011.
- dr Dean R. Evans, Air Force Research Laborathory, Ohio, USA, 07-11 March 2011. 4
- 5. Maria Filkusová, Dept. of Physical Chemistry, University of P.J.Safarik in Kosice, Kosice, Slovakia, 02 April to 31 July 2011.
- 6. Anna Pogrebna, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, 30 May to 06 June 2011.
- 7. Samuel Ainsley Varley, Heriot Watt University, Edinburgh, Great Britain, 1 June to 31 July 2011.
- 8. prof. Feodor Kusmartsev, Department of Physics, Loughborough University, Loughborough, Great Britain, 13-16 June 2011.
- dr Owain Parri, Merck Chemicals, Great Britain, 27-28 June 2011.
- 10. dr Rachel Tuffin, Merck Chemicals, Great Britain, 27-28 June 2011.
- 11. prof. Geoffrey Luckhurst, Merck Chemicals, Great Britain, 27-28 June 2011.
- 12. Ivan Madan, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, 05-11 July 2011.
- 13. prof. Mikael Hedenqvist Department of Fibre and Polymer technology, KTH School of Chemical Science and Engineering, Stockholm, Sweden, 03-17 July 2011
- 14. Igor Vaskivskyi, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, 24-27 July 2011.

- 15. dr Yasunori Toda, Department of Applied Physics, Hokkaido University, Sapporo, Japan, 26-29 July 2011.
- 16. Michael Treber, Omicron NanoTechnology GmbH, Taunusstein, Germany, 14-15 September 2011.
- 17. dr Claudio Giannetti, Universitr Cattolica del Sacro Cuore, Dipartimento di Matematica e Fisica, Brescia, Italy, 28-29 September 2011.
- 18. Sergii Shelestiuk, Physics Faculty, National Taras Shevchenko University of Kyiv, Kyiv Ukraine, 30 September to 13 November 2011.
- prof. Srdanov Vojislav, Institute of Physics, Belgrade and the Institute for Terahertz Science and Technology, University of California at Santa Barbara, Santa Barbara, California, 17 October 2011.
- 20. dr Wei Li, TEDA Applied Physics School, Tianjin, China, 03-10 December 2011.
- 21. asst. prof. Giusy Scalia, Graduate School of Convergence Science and Technology Seoul, Seoul, Korea, 04-11 December 2011.
- 22. prof. Andras Kis, Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland, 19-20 December 2011.

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24. Dr. Miha Devetak, left 01.07.11

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- 31. Dr. Jure Strle
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#### PATENT APPLICATION

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# 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

Our research in the field of reactor physics was continued on the development of new methods for analysing research and power reactors. With the colleagues from CEA-Cadarache a series of measurements was performed on the TRIGA reactor. The spatial distribution of the fission-reaction rate in the core was accurately measured. New neutron dosimeters and self-powered detectors were tested. The results will serve for a validation and improvement of computational models and an improvement of the accuracy of the absolute power calibration in the TRIGA reactor.

We also studied the resonance self-shielding effects and came across an interesting observation, according to Head: which the propagation of uncertainties from the basic data to the integral observables can sometimes increase **Asst. Prof. Andrej Trkov** significantly when strong self-shielding is present, but to obtain accurate results it is necessary to start from the covariances of the resonance parameters, rather than from the derived covariances of the cross-sections.

Through international collaboration we continued the work on the nuclear-data evaluation. Evaluations for six materials were accepted into the latest US-evaluated nuclear-data library ENDF/B-VII.1, which was released in December 2011.



In the field of **plasma physics** further knowledge was acquired in the theory of electron-emitting floating electrodes immersed in a complex plasma. The research area corresponds well with the development of plasma diagnostics inside fusion devices. To improve the analytical and numerical models, particle-in-cell (PIC) codes have been successfully used in the research of the saturation of the floating potential for an emissive probe in the cases

when the temperature of the emitted electrons is close to the temperature of the bulk electrons. The transitions between the temperature-limited and space-charge-limited emissions were studied carefully. We have also finished the first round of the planar emissive probe simulations in a midsized tokamak. Two articles discussing the above issues were published. A new field of research was opened by studying the Townsend discharge via the PIC simulations intending to support the gas discharge tubes as the surge protection devices. In collaboration with Bulgarian INRNE.BG a series of experiments was started on our linear plasma device to measure the distribution functions of the negative ions in a magnetized plasma with a Langmuir probe. In addition, the first use of the so-called "ball-pen" probe in our linear plasma device was made in collaboration with Czech IPP.CZ. The results obtained were used for a calibration of this type of probe before its installation in the tokamak ASDEX-UPGRADE.

panded our collaboration with the Joint European Torus (JET), the largest fusion reactor in the world. Researchers of the Reactor Physics Department have made longer visits to JET in order to make calculations of the response shielding and absorption. of the in-vessel neutron detector and, in this way, improve its calibration.



In the field of neutron transport calculations we continued and ex- Figure 1: Calculated effect of the JET remote handling system on the neutron-flux distribution in the JET tokamak. The green colour denotes the area where the effect is insignificant, i.e, less than 3 %, blue denotes the area where the neutron flux is decreased by 20-30 %, mainly due to

The work was necessary after the change of the torus first wall to beryllium in view of the change in the neutron field. The IJS staff is co-responsible for the maintenance of the JET model for transporting the calculations with the Monte Carlo method and, in 2011, our model was expanded in order to cover the whole torus. The existing model covers only one quarter of the torus, making use of the reflecting boundary conditions. The new model can also be used for point sources and is applicable for calibration purposes.

We also collaborate on the project of neutron-detector calibration. Our tasks are transport calculations for the determination of calibration uncertainties and determination of corrections arising from the operating conditions, which differ from the conditions during a calibration, e.g., in-vessel structures, neutron spectra, neutron source shape, etc. In 2011 our work was especially devoted 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 by calculating the neutron cross-talk between the collimator channels of the KN3 neutron camera. It turned out that the required correction arising from the cross-talk is small, as experimentally predicted in the 1980s. However; the calculations provided a much better insight into the origin and the locations of the scattered neturons and a better understanding of the phenomenon of the cross-talk through the KN3 concrete shield.

In the course of investigating organic semiconductors as possible **radiation detectors for low-energy neutrons** an analytical proof has been given that the electric field at the metal/organic semiconductor, the crucial a-priori assumption of the mathematical description of the current-voltage relationship through such structures,



Figure 2: Response assessment for a targeted therapy. Response is assessed using the FLT PET/CT imaging before the start of the therapy (Scan #1), after two weeks of the therapy (Scan #2) and at the end of the first cycle of the therapy – two weeks on therapy, one week off therapy (Scan #3). The upper row shows quantification with an optimized kinetic analysis and the K<sub>1</sub> parameter (a radiopharmaceutical tissue uptake). The lower row shows the Standardized Uptake Value (SUV). It is obvious from the figure that the image quantification seriously affects the response assessment.

cannot vanish. Using a set of published current-voltage data as obtained on the electron-only ITO/OC<sub>1</sub>C<sub>10</sub>-PPV(220 nm)/Yb, and electron-only Al/MEH-PPV(270 nm)/Ba organic structures, it is shown that the Mark-Helfrisch model of the charge transport in the presence of the traps exponentially distributed within the organic is, for the above reason, incomplete and thus inaccurate. Our study has confirmed that: (a) the metal/organic interfacial charge density is indeed non-zero and from the current-voltage data it is currently possible to deduce only an interval of the trap charge densities that is compatible with the data specific to each organic structure, (b) the internal electric field at the midpoint of the organic layer turns out to be unique in the sense that it is equal to the externally applied electric field, (c) this location is being characterized by the minimum trap charge density, and (d) the bias dependence of the corresponding free charge density at this particular position is well approximated in terms of an exponential function of the external bias voltage.

Our research in the field of **medical physics** is directed towards the image-guided cancer therapy. Within this general area, we are focused mainly on the quantitative PET imaging. The quantification is based on the kinetic analysis of the radiopharmaceutical tissue uptake. The kinetic analysis is done at the voxel level, which allows a parametric image generation and

the following spatial distribution of a disease progress and a response to therapy. The topics of our research are the optimization of the kinetic-analysis method, an assessment of the kinetic-analysis results uncertainty, and the usage of the kinetic-analysis methods in clinical studies. The usage of the PET-image kinetic analysis allows us to quantify the basic processes traced by the radiopharmaceutical used, and to quantify the vasculature status and the amount. In addition, our research in the quantitative PET imaging is focused on the assessment of the other uncertainties related to PET imaging, e.g., an impact of a patient set-up and motion on the quantification of PET images. As part of the image-guided cancer therapy we do some research in imaging for biological target definition, imaging for the treatment assessment, modelling of tumour growth and response to therapies, and open-source medical devices.

#### Some outstanding publications in the past year

- 1. Chadwick M.B., Trkov Andrej. ENDF/B-VII.1 nuclear data for science and technology: cross sections, covariances, fission product yields and decay data. *Nucl. data sheets (N.Y. N.Y.)*, 2011, no. 12, vol. 112, pp. 2887-2996.
- Trkov Andrej, Capote R., Soukhovitskii E., Leal L.C., Sin M., Kodeli Ivan Aleksander, Muir D.W. Covariances of evaluated nuclear cross section data for <sup>232</sup>Th, <sup>180, 182, 183, 184, 186</sup>W and <sup>55</sup>Mn. *Nucl. data sheets (N.Y. N.Y.)*, 2011, iss. 12, vol. 112, pp. 3098-3119.
- Žerovnik Gašper, Trkov Andrej, Capote R., Rochman D. Influence of resonance parameters correlations on the resonance integral uncertainty, <sup>55</sup>Mn case. *Nucl. instrum, methods phys res., Sect. A, Accel.*. [Print ed.], 2011, vol. 632, issue 1, pp. 137-141, doi: 10.1016/j.nima.2010.12.210.
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- Liu G., Jeraj Robert, Vanderhoek M., Perlman S., Kolesar Jill M., Harrison M.R., Simončič Urban, Eickhoff J.C., Carmichael L., Chao B., Marnocha R., Ivy P., Wilding G. Pharmacodynamic Study Using FLT PET/CT in Patients with Renal Cell Cancer and Other Solid Malignancies Treated with Sunitinib Malate. *Clin Cancer Res*, 17(24), 2011, 7 pp., doi: 10.1158/1078-0432.CCR-11-1677.

#### Organization of conferences, congresses and meetings

1. Nuclear Society of Slovenia: Young Generation Network Internal Conference, Milan Čopič Nuclear Training Centre, Jožef Stefan Institute, Brinje, Slovenia, 23.11.2011 (organizer/chair of the first section: Gašper Žerovnik, chair of the second section: Luka Snoj, 13 participants, 10 contributions)

## INTERNATIONAL PROJECTS

- 1. Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN FUSEX EURATOM – MHEST
  - 7. FP EURATOM, Slovenian Fusion Association SFA
  - 3211-08-000102, FU07-CT-2007-00065
  - EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Igor Lengar, Melita Lenošek Kavčič, B. Sc., Tomaž Skobe, B. Sc., Asst. Prof. Saša Novak Krmpotič
- 2. Accurate Nuclear Data for Nuclear Energy Sustainability
- ANDES,

3.

7. FP - EURATOM, 249671

#### EC; Dr. Enrique Miguel Gonzalez Romero, Centro de Investigaciones Energeticas, Medioambientales y Tecnologicas-CIEMAT, Madrid, Spain Asst. Prof. Andrej Trkov

- Improvement of Diagnostics in Edge Plasmas of Fusion Devices 1.2.1.-FU
- EURATOM MHEST
- 7. FP EURATOM, Slovenian Fusion Association SFA
- 3211-08-000102, FU07-CT-2007-00065
- EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Tomaž Gyergyek
- Upgrade of Gamma-Ray Cameras: Neutron Attenuators 2.2.1. FU
   F.P EURATOM, Slovenian Fusion Association SFA
   3211-08-000102, FU07-CT-2007-00065, JW6-TA-EP2-GRC-02, JW8-NEP-MHST-02
   EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Igor Lengar
- Neutron Calculation for Fusion Reactor Neutron Source 3.4.2.-FU JW11-FT-5.35/JW11-NFT-MHEST, EURATOM – MHEST
   FP - EURATOM, Slovenian Fusion Association – SFA 3211-08-000102, FU07-CT-2007-00065
   EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia
  - Dr. Luka Snoj
- Neutron Calculations for Fusion Reactor JET MCNP Model 3.4.1.-FU10 Agreement TA JW11-FT-JET-5.34/JW10-NFT-MHST-04 EURATOM - MHEST
- 7. FP EURATOM, Slovenian Fusion Association SFA
- 3211-08-000102, FU07-CT-2007-00065
- EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Igor Lengar
- Neutron Calculations for Fusion Reactor JET MCNP Model 3.4.1.-FU11 Agreement TA JW11-FT-JET-5.36/JW11-NFT-MHST, EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association - SFA 3211-08-000102, FU07-CT-2007-00065
- EC, RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Igor Lengar
- Research Unit Administration and Services RU-FU EURATOM – MHEST
  - 7. FP EURATOM, Slovenian Fusion Association SFA
  - Annex 3, 3211-08-000102, FU07-CT-2007-00065
  - EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Prof. Milan Čerček, Asst. Prof. Saša Novak Krmpotič
- 9. F4E Action 2 Nuclear Data Experiments and Techniques ACTION F4E-GRT-056 (ES-AC)
  - ACTION 2

Dr. Paola Batistoni, ENEA - Agenzia nazionale per le nuove tecnologie l´energia e lo sviluppo economico sostenibile, Frascati (Rome), Italy Dr. Ivan Aleksander Kodeli

MENTORING

#### Ph. D. Thesis

1. Urban Simončič, Modeling of radiopharmaceuticals uptake into the tumor : optimization of the method and its applicatiom in the clinical studies (mentor Robert Jeraj).

 Working Group 6 - Conrad: Computational Dosimetry, Task on Standard Monte Carlo Modelling of a Medical Linac (Priority 2), Subtask: Uncertainty Assessment for Radiation Dosimetry (Priority 3) EURADOS

G. Gualdrini, ENEA - Italian National Agency for New Technologies, Energy and Sustainable Economic Development, Montecuccolino Laboratories, Bologna, Italy Dr. Ivan Aleksander Kodeli

 Evaluation and Validation of Promt Fission Neutron Spectra and the Corresponding Covariance Matrices 15794/R0

Teresa Ann Benson, IAEA - International Atomic Energy Agency, Vienna, Austria Dr. Ivan Aleksander Kodeli

- Improvement of Evaluated Nuclear Data Files with Emphasis on Activation and Dosimetry Reactions; Nuclear Data Libraries for Advanced Systems: Fusion Devices (FENDL-3)
  - 14914/R0, R1, R2 Nathalia Calinat, IA

Nathalie Colinet, IAEA - International Atomic Energy Agency, Vienna, Austria Asst. Prof. Andrej Trkov

 Research and Development of Plasma Diagnostic Techniques with Emissive Probe Untersuchungen und Entwicklung diagnostischer Methoden mit Emissiven Sonden BI-AT/11-12-023

Dr. Cordina Ioniță-Schrittwieser, Institute for Ion Physics and Applied Physics, Leopold-Franzens-University of Innsbruck, Innsbruck, Austria Prof. Milan Čerček

# R & D GRANTS AND CONTRACTS

- 1. A study of plasma parameters for conditioning of the inner surfaces of a fusion reactor Prof. Miran Mozetič
- Functionalization of biomedical samples by thermodynamic non-equilibrium gaseous plasma Prof. Miran Mozetič
- Calculations to support neutron monitor calibration JET fusion reactor example case Dr. Luka Snoj

## RESEARCH PROGRAM

1. Reactor Physics Asst. Prof. Dr. Andrej Trkov

## NEW CONTRACTS

- Criticality safety analysis of the NPP Krško spent fuel in the disposal facility at nominal conditions
  - ARAO Agency for Radwaste Management Dr. Marjan Kromar
- Reload Operational Core Analysis, Post Refueling Nuclear Design Check Test.. Nuclear Power Plant Krško Dr. Marian Kromar

### VISITORS FROM ABROAD

- 1. Dr. Codrina Ionita Schrittwieser and prof. dr. Roman Schrittwieser, Institute for Ion Physics, University of Innsbruck, Austria, 17.7. – 30.7.2011
- Hannes Gruenwald, Institute for Ion Physics, University of Innsbruck, Austria, 31.7. 12.8.2011
- Prof. Tsviatko Popov, Faculty for Physics, University "St. Kliment Ohridski", Sofia, Bulgaria, 3.5. - 13.5.2011

- 4 Ana Bankova and Mladen Mitov, Faculty for Physics, University »St, Kliment Ohridski«, Sofia, Bulgaria, 3.5. - 27.5.2011
- Prof. Sean Fain, University of Wisconsin, Wisconsin, Madison, USA, 25.10. 3.11.2011 6. Dr. Christophe Domergue, dr. Loic Barbot and dr. Gilles Gregoire, CEA, Cadarache, France, 3.10. - 14.10.2011

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- Prof. Bruno Cvikl\*, left 01.10.11
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- Prof. Robert Jeraj 4.
- Dr. Ivan Aleksander Kodeli
- 6. Dr. Marjan Kromar
- Dr. Igor Lengar

#### 8. Asst. Prof. Andrej Trkov, Head Asst. Prof. Tomaž Žagar\*, left 10.10.11

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- 10. Dr. Luka Snoj
- Postgraduates

#### 11. Dušan Ćalić, B. Sc.

12. Vladimir Radulović, B. Sc.

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- 8 Dr. Roberto Capote Noy, International Atomic Energy Agency, Vienna, Austria, 18.12.-24.12.2011
- 13. Dr. Urban Simončič 14. Gašper Žerovnik, B. Sc. **Technical officers** 15. Alberto Milocco, M. Sc. Technical and administrative staff 16. Dušan Rudman 17. Slavko Slavič, B. Sc. 18. Darinka Stich 19. Uršula Turšič, B. Sc. 20. Bojan Žefran

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#### **RESEARCH MONOGRAPH**

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#### PH. D. THESES

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# 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, which are required for such measurements. Astroparticle physics is an emerging field applying experimental techniques of particle physics to solve astrophysical problems. Slovenian researchers are participating in the measurements of the ultra-high-energy cosmic rays with the Pierre Auger Observatory spread over a surface of 3000 km<sup>2</sup> 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 where they are affordable only as joint international enterprises. Thus, future accelerators will be unique facilities Head: of their kind, the first being the Large Hadron Collider (LHC), just completed at the European Organization for Prof. Marko Mikuž 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 remain 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 at 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 km<sup>2</sup>) observatory near Malargue in Argentina for detecting ultra-high-energy cosmic rays. This endeavour is carried out in collaboration with the colleagues from the University of Nova Gorica.

A more detailed report on the 2011 activities follows, focused on the contributions of our researchers:

#### **ATLAS experiment**

The operation of the Large Hadron Collider (LHC) at CERN, during 2011, exceeded the most optimistic expectations. The frequency of collisions was increased by a factor of 15 compared to 2010 and the operation was stable even at the highest frequency. Two large experiments, ATLAS and CMS, allowed an analysis of the data from a sample of integrated luminosity of 5 fb<sup>-1</sup>. This is a factor of 5 beyond the LHC predictions at the beginning of 2011 and by a factor of 100 higher than the luminosity in 2010.

The Slovenian group of ten scientists is involved in the ATLAS collaboration joining the efforts of more than 3000 scientists. The collaborators analysed the collected data on a global network based on the Grid technology, and the Slovenian contribution to the data processing was significant. Figure 1: Integrated luminosity in 2011 recorded by the ATLAS

The results of the physical analysis were presented in more than 100 experiment scientific papers submitted for publication in the most prestigious scientific

journals. Among them, the measurement of the total cross-section for the scattering of protons at 7 TeV was published in Nature Communications. The scientific community showed great interest in the analysis search for new particles predicted by the theories extending the standard model. So far, these particles have not been found and

the existence of the Higgs Boson with a mass of about 126 GeV.



The results of the ATLAS experiment indicate





higher, upper limits for masses were set. Some of the simplest supersymmetrical models have been already excluded by taking into account the experimental results.

The amount of the collected data allowed us to accelerate significantly the search for the Higgs Boson, the last undiscovered particle of the Standard Model. Preliminary results of the analysis of decays with the highest predictive power have enabled us to exclude the Higgs particle masses practically across the whole range except for a narrow



Figure 2: Measurements exclude the existence of the Higgs Boson with a mass larger than 131 GeV and indicate its existence with a mass of around 126 GeV.

interval between 115 and 131 GeV. In this interval we have observed excess of events above the background around 126 GeV. This excess is consistent with the probability of the occurrence of the Higgs Boson in the Standard Model. However, the probability of fluctuations in the background is still too high to unambiguously confirm its existence. We expect that the fluctuations in the background will decrease and we will be able to confirm or disregard the existence of the Higgs Boson. The existence of the Higgs Boson in this mass interval allows an in-depth study of its properties, which are sensitive to the signals originating from the extension of the Standard Model.

The SiGNET Tier-2 grid site has increased its computing capacity to 2000 cores and 800TB of data storage space in the year 2011. As a constitutive member of the Slovenian National Grid Initiative, SLING/NGI, the site had supported and maintained the Slovenian grid infrastructure together with Arnes. Two new clusters, one at the University of Nova Gorica and the other at the CIPKEBIP, had joined the Slovenian grid infrastructure. The SiGNET is a full member of international organizations EGI/InSPIRE, wLCG and Nordugrid and had participated in several joint projects related to the support, maintenance and planning of the computing infrastructure as well as the development, distribution and deployment of the grid middleware. The main

objective of the SiGNET Tier-2 is to support the data processing and storage for the international experiments ATLAS, Belle and Pierre Auger. In addition, the site provides support to Slovenian research and educational organizations.

#### Belle detector at the asymmetric electron-positron collider KEKB at KEK

One of the important unsolved questions of modern science is why we are living in a universe in which matter (particles) totally dominates over antimatter (antiparticles). The necessary condition for this to happen is the violation of the CP symmetry, which can be measured in the world of elementary particles as the difference between the decays of particles and their antiparticles. In more than a decade of measurements of the violation of

After the accurate measurements of the CP symmetry violation in the B meson system, the Belle Collaboration has performed a series of measurements of extremely rare processes, which limit the set of models used to describe the so-called New Physics. These processes will be examined with a much greater accuracy with the Belle II detector that will start its operation in 2015. The observation of the tetraquark states is a breakthrough in the hadron spectroscopy. the CP symmetry in the B meson system with the Belle detector at the KEKB collider, the predictions of the Kobayashi-Maskawa model, which theoretically describes the CP violation, were accurately confirmed, for which the Japanese theorists received the Nobel Prize for Physics in 2008. It also became clear that the observed asymmetry between particles and antiparticles is too small to explain the dominance of matter over antimatter in the Universe. Hence, there must exist as yet unknown particles and processes, which are popularly known as New Physics (NP). The purpose of the latest extremely accurate measurements using the data recorded by the Belle detector, which stopped its operation in July 2010, and the planned measurements with the upgraded collider SuperKEKB and the Belle II detector, which are expected to start taking data in 2015, is the search and the identification of the NP processes. One of the hot topics in this area of physics is certainly the search

for the CP violation in D meson decays. In 2011, we finalized a measurement of a CP asymmetry in D<sup>0</sup> meson decays into the phi meson and a charged pion [3]. The measured upper limit for the CP asymmetry in this decay allows us to constrain several parameters of the models describing the NP processes. In 2011 there was also an important breakthrough in hadron spectroscopy, from a set of measurements that help to reveal the nature of the exotic X(3782) [4] to a discovery of two states that correspond to, up to now, unobserved bound states of four quarks, the so-called tetraquark. In 2011 we also passed another important milestone, a ground-breaking ceremony of the Belle II experiment, an international project with 400 physicists where the Slovenian physicists play a leading role.

#### **Pierre Auger observatory**

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 (UHECR). Constructed in the province of Mendoza, Argentina, the observatory is the first hybrid air-shower experiment combining two independent observation techniques.

It consists of a 3000 km<sup>2</sup> array 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). These two detectors measure, in a complementary way, the extensive air showers initiated by primary cosmic rays. The longitudinal development of the air showers in the atmosphere is measured directly with the FD. It has a better energy resolution and well-understood energy systematics, while the SD has larger statistics and a well-defined aperture. In addition, the depth of the maximum development of the showers is measured with the FD. This observable encodes information about the composition of the primaries and about the properties of the first hadronic interactions. The Pierre Auger Observatory started taking data in January 2004 with only 100 water Cherenkov detectors and one fluorescence telescope and has been operating continuously since then. The construction of the Observatory was completed in mid 2008.

Above 10<sup>9</sup> eV, the cosmic ray flux falls with energy E, roughly as  $E^{\gamma}$  where the spectral index  $\gamma \sim 3$ . Several breaks in the spectral index have been observed presumably reflecting some property of the cosmic-ray propagation or acceleration. Two of these spectral features appear in the energy region

currently accessible to the Auger Observatory. Last year an updated Auger measurement of the energy spectrum was published. This measurement uses both hybrid and SD-only events. The collaborators reported a suppression of the flux with  $\gamma = 2.59\pm0.02$  and  $\gamma = 4.3\pm0.02$  below and above  $\log(E)=19.46\pm0.01$ , respectively. These observations are consistent with the predictions of Greisen, Zatsepin and Kuzmin (GZK), who noted that above  $\sim 10^{20}$  eV, cosmic rays should interact strongly with the cosmic microwave background (CMB) radiation, leading to a degradation in the cosmic-ray energy. The second change in the spectral index, known as the "ankle", occurs at an energy of about  $\log(E)=18.61\pm0.01$  with  $\gamma = 3.2\pm0.04$ . This feature may be a result of a steep spectrum from galactic sources crossing over a flatter spectrum from extragalactic sources.

The measurement of the cosmic-ray mass composition provides a crucial input for understanding the sources and propagation of the cosmic rays at ultra-high energies. For instance, the variation of the composition with energy may shed light on what mechanism is responsible for the ankle, and help to clarify whether the flux suppression is

due to the GZK effect or a limitation of acceleration mechanisms. Because of the indirect techniques necessary to detect and study the UHE cosmic rays, through their atmospheric cascades, a direct determination of the primaryparticle type is not possible. However, the evolution of air showers in the atmosphere is expected to be statistically different, on average depending on the type of the primary particle. At a given primary energy, more massive particles yield showers that develop sooner, for which the depth of the



Given that the highest energy cosmic rays observed should exhibit trajectories which 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 the cosmic rays with the energies near  $10^{20}$  eV would not be seen. Since the matter density within about 100 Mpc is not isotropic, this compounds a potential for anisotropy to emerge in the UHECR sample. Using the Auger data, both point source studies have been performed as well as a harmonic analysis of arrival directions, which characterize anisotropy at various angular scales. Based on the Auger data set, 21 out of 55 events with energies higher than 5.6 x  $10^{19}$  eV were found to be correlated with the objects in the Veron-Cetty catalog of active galactic nuclei. The strength of the correlation is smaller than previously published. However, evidence for anisotropy remains in the sense that there is a 0.3% chance to find 21 or more of 55 events from an isotropic distribution that correlate with a catalog object subject to the cuts on the source opening angle and redshift. Correlations on such a small angular scale as those reported  $(3.1^{\circ})$  would seem to be at odds with the apparent trend to heavy composition at a high energy, since heavier nuclei would be more deflected by intergalactic and galactic magnetic fields.



Figure 3: Discovery of a tetraquark state with the Belle spectrometer: the mass of a particle decaying into a charged pion and the Upsilon(1s) resonance, a bound state of a b quark and its anti-quark.

The measurements of the Pierre Auger experiment support the reduced correlation between the mass distribution in the Universe and the direction of the cosmic rays.





Figure 5: Image of the phantom taken with a conventional PET (Fig. 5a) and with a PET Si probe (Fig. 5b)

#### **Detector development**

In 2011 we based the detector development on a successful measurement with a silicon photomultiplier detector module. We created a new type of apparatus for positron tomography (PET) and measured its energy and time resolution. Such a counter is an extremely interesting candidate for the dual-modality medical imaging, where a PET apparatus is embedded in an MRI imager, and the light sensors have to operate in magnetic fields exceeding 2 T. This research is a part of an EU 7FP research project aimed at the development of novel detection methods for particle physics and medical imaging. In preparation for the next generation of the measurements of rare phenomena in B mesons decays with the Belle II spectrometer, we continued the study of the sensors for two ring-imaging Cherenkov detectors. In collaboration with the leading producers in this area, Hamamatsu (Japan) and Photonis (France), we studied the characteristics of the photomultiplier tubes with micro-channel plates and the hybrid photon detectors with avalanche

photodiodes like for photoelectron detectors.

We have developed a new method that has a potential to revolutionize positron emission tomography (PET), one of the most important medical imaging techniques. We have, namely, shown that the detection time of the annihilation gamma rays can be measured with an accuracy of 40ps (Fig. 4) if the conversion medium is a Cherenkov radiator rather than a scintillator, and if the resulting Cherenkov photons are detected with a microchannel-plate photomultiplier tube (MCP PMT) [5]. This is a very important result; by measuring the difference of detection time of both gamma rays one can very accurately determine the annihilation point along the line connecting both detectors. With such a detector one could improve the imaging properties of a PET apparatus. The study had a lot of response in the scientific community and was invited for presentation in the most prestigious session of the IEEE NNS/MIC conference, the main conference for nuclear detectors and imaging.

In collaboration with CERN, University of Valencia, University of Michigan, Ann Arbor and State University in Ohio, we carried out the measurements of the new PET system improved with the position-sensitive silicon detectors. We took pictures with the test phantom and measured the spatial resolution of PET.

We continued with the development of silicon detectors that operate in high-radiation fields [6]. By measuring the signal generated with an infrared laser beam with a side impact on the detector, we measured the electric field in the silicon sensors. We irradiated detectors at the Reactor Centre in Podgorica up to the fluences of  $10^{16}$  cm<sup>-2</sup> and measured the position dependence of the signals. The existence of a charge multiplication near the electrodes was confirmed.

Within the European project AIDA (Advanced Infrastructures European for Detectors at Accelerators) we performed more than 100 irradiations with neutrons at the Reactor Center in Podgorica. In the first year of this project the focus was on the preparations for the construction of a new inner-layer detector in the ATLAS spectrometer (Inner B-Layer).

#### Awards and appointments

1. Zois Award for lifetime achievements in physics, Academician Prof. Gabriel Kernel

#### Organization of conferences, congress and meetings

1. Workshop "4th Belle II Computing Workshop", 23. 5. 2011 - 25. 5. 2011, Jožef Stefan Institute, Ljubljana, Slovenia

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## INTERNATIONAL PROJECTS

1. Advanced European Infrastructures for Detectors at Accelerators AIDA 7. FP, 262025 EC; Svetlomir Stavrev, European Organization for Nuclear Research, CERN, Geneva, Switzerland Prof. Marko Mikuž 2 European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe EGI-InSPIRE 7. FP, 261323 EC; The Stichting European Grid Initiative, Amsterdam, The Netherlands; Academic and Research Network of Slovenia - ARNES, Ljubljana, Slovenia Prof. Marko Mikuž 3. Improving Access to Text IMPACT 7. FP, 215064 EC; Hildelies Balk, Koninklijke Biblioteek, Haag, The Netherlands Jan Jona Javoršek, B. Sc., Asst. Prof. Tomaž Erjavec Marie Curie Training Network on Particle Detectors MC-PAD 7. FP, 214560, PITN-GA-2008-214560 EC; Seamus Hegarty, CERN, Geneva, Switzerland Prof. Peter Križan Joint Research on Various Types of Radiation Dosimeters 5 RADDOS 7. FP, 207122 EC; University College Cork, National University of Ireland, Tyndall National Institute, Cork, Ireland Dr. Gregor Kramberger Enabling Grids for E-sciencE III 6 EGEE-III EGEE-SA1, EGEE-NA2, EGEE-NA4 7. FP, 222667 EC; Dr. Bob Jones, Anna Cook, CERN IT-EGE, Geneva, Switzerland Prof. Marko Mikuž Collaboration DELPHI Dr. Jan Timmermans, CERN, Geneva, Switzerland Prof. Borut Paul Kerševan Collaboration ATLAS Prof. Peter Jenni, Dr. Fabiola Gianotti, CERN, Geneva, Switzerland Prof. Marko Mikuž Collaboration CERN RD-39 Dr. Jaako Haarkonen, Helsinki Institute of Physics (HIP), University of Helsinki, Helsinki, Finland Dr. Zheng Li, Brookhaven National Lab (BNL), Upton, NY, USA Prof. Marko Mikuž 10. Collaboration CERN RD-42 Prof. Peter Weilhammer, CERN, Geneva, Switzerland Prof. Marko Mikuž

### **MENTORING**

#### Ph. D. Thesis

1. Boštjan Maček, Measurement of luminosity in ATLAS spectrometer with beam conditions monitor (mentor Marko Mikuž; co-mentor Andrej Gorišek).

## VISITORS FROM ABROAD

- Prof. Ichiro Adachi, KEK, Tsukuba, Japan, 2. 3. 2011 5. 3. 2011
   Dr. Shohei Nishida, KEK, Tsukuba, Japan, 21. 3. 2011 6. 3. 2011
- Philipp Weigell, BSc in Physics; Institut Max Planck, Muenchen, Germany, 23. 3. 2011 -3. 25. 3. 2011; 29. 7. 2011 - 4. 8. 2011; 12. 12. 2011 - 16. 12. 2011

- 11. Collaboration CERN RD-50 Prof. Mara Bruzzi, University of Florence, Florence, Italy Dr. Michael Moll, CERN, Geneva, Switzerland Prof. Marko Mikuž
- 12. Collaborations Belle in Belle II Prof. Masanori Yamauchi, KEK, Tsukuba, Japan Prof. Peter Križan
- 13. Collaboration CIMA; Cameras for Imaging in Medical Applications Prof. Peter Weilhammer, CERN, Geneva, Switzerland Prof. Marko Mikuž
- 14. Measurements of Mixing and CP Violation in DO System BI-JP/10-12/A-003 Prof. Sokai Yoshihide, High Energy Accelerator Research Organization, KEK, Tsukuba, Ibaraki, Japan
- Prof. Boštjan Golob 15. Development of New Detectors for PET Imaging BI-US/09-12-042 Prof. Neal Clinthorne, University of Michigan, Dept. of Radiology, Ann Arbor, MI, USA Prof. Mikuž Marko

### **R &D GRANTS AND CONTRACTS**

- 1. Tracking system for particles in test beam setupsá
- Dr. Andrej Gorišek Measurements of Mixing and CP Symmetry Violation in D^0 Meson System 2 Prof. Boštian Golob
- Particle detectors at future generation colliders 3. Prof Marko Mikuž
- Development of solid state detectors for particle physics experiments 4 Prof. Vladimir Cindro
- 5 Gridification of Particle Physics Data Analysis: A Pilot Project of Slovenian National Grid Initiative Prof. Marko Mikuž
- 6. Measurement of the absolute branching fractions of leptonic D(s) decays and the extraction of the decay constant f\_D(s) Dr. Anže Zupanc

### RESEARCH PROGRAMS

- Astroparticle Physics
- Asst. Prof. Marko Zavrtanik
- **Experimental Particle Physics** Prof. Marko Mikuž
- Prof. Leo Piilonen, Virginia Polytechnic Institute and State University, Blacksburg, 4. Virginia, USA, 23. 5. 2011 - 25. 5. 2011
- 5. Prof. Takanori Hara, High Energy Accelerator Research Organization (KEK), Tsukuba, Japan, 23. 5. 2011 - 25. 5. 2011
- Prof. Ki Hyeon Cho, Korea Institute of Science and Technology Information (KISTI), 6 Daejeon, Korea, 23. 5. 2011 - 25. 1. 2011
- 7. Shuichi Iwata, BSc in Physics, Tokio Metropolitan University, Tokio, Japan, 19. 8. 2011 - 16. 9. 2011
- 8. Prof. Dr. Goran Ristić, Faculty of Electronic Engineering, Univesity of Niš, Serbia, 18.9. 2011 - 1 10 2011
- Mimoir Todorović, Bachelor of Engineering, Faculty of Electronic Engineering, Univesity of Niš, Serbia, 2. 10. 2011 23. 12. 2011 9.
- 10. Prof. William Barletta, editor of NIMA, 20. 10. 2011
- Graeme Stewart, BSc in Physics, University of Glasgow, Scotland, 2. 11. 2011 20. 11. 11 2011
- 12. Prof. Dr. William Trischuk, University of Toronto, Toronto, USA, 18. 11. 2011

### STAFF

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- Prof. Boštjan Golob\* 4. Dr. Andrej Gorišek
- 6. Prof. Borut Paul Kerševan\*
- Prof. Samo Korpar\*
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- 13. Asst. Prof. Tomaž Podobnik\*
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- 16. Asst. Prof. Marko Zavrtanik
- 17. Prof. Danilo Zavrtanik\* 18. Asst. Prof. Dejan Žontar\*

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- 20. Asst. Prof. Marko Bračko\*
- 21. Dr. Andrej Studen
- 22. Dr. Matevž Tadel, left 01.04.11

#### 23. Dr. Anže Zupanc Postgraduates

- 24. Jyoti Prakash Biswal, B. Sc.
- 25. Maksym Deliyergiyev, B. Sc.

## BIBLIOGRAPHY

27. Milan Grkovski, B. Sc 28. Jure Klučar, B. Sc. 29. Marko Kobal\*\* 30. Dr. Boštjan Maček 31. Marko Milovanović, B. Sc. 32. Marko Petrič, B. Sc. 33. Eva Ribežl, B. Sc. 34. Peter Smerkol, B. Sc. 35. Andrej Seljak\* 36. Luka Šantelj, B. Sc 37. Elvedin Tahirović, B. Sc. 38. Andrii Tykhonov, B. Sc. 39. Ruben Verheyden, B. Sc. **Technical officers** 40. Andrej Detela, B. Sc. 41. Borut Grošičar, B. Sc. 42. Jan Jona Javoršek, B. Sc. Technical and administrative staff 43. Andreja Butina 44. Jurij Eržen 45. Dejan Lesjak 46. Erik Margan

26. Rok Dolenec, B. Sc.

#### Note:

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#### ORIGINAL ARTICLES

- 1. ATLAS Collaboration: G. Aad et al. (3035 authors), "Inclusive search for same-sign dilepton signatures in *pp* collisions at  $\sqrt{s} = 7$ TeV with the ATLAS detector", J. high energy phys., vol. 2011, no. 10, pp. 107-1-107-48.2011.
- 2. ATLAS Collaboration: G. Aad et al. (3022 authors), "Measurement of the  $Z \rightarrow \tau \tau$  cross section with the ATLAS detector", *Phys. rev., D Part.* fields gravit. cosmol., vol. 84, no. 11, pp. 112006-1-112006-29, 2011.
- 3. ATLAS Collaboration: G. Aad et al. (3027 authors), "Measurement of the  $\gamma(1S)$  production cross-section in *pp* collisions at  $\sqrt{s} = 7$ TeV in ATLAS", Phys. lett., Sect. B, vol. 705, no. 1/2, pp. 9-27, 2011.
- 4. ATLAS Collaboration: G. Aad et al. (3014 authors), "Measurement of the inclusive and dijet cross-sections of *b*-jets in *pp* collisions at  $\sqrt{s}$  = 7TeV with the ATLAS detector", *The European physical journal. C*, vol. 71, no. 12, pp. 1846-1-1846-22, 2011.
- 5. ATLAS Collaboration: G. Aad et al. (3026 authors), "Measurement of the inclusive isolated prompt photon cross-section in pp collisions at  $\sqrt{s} = 7$ TeV using 35  $pb^{-1}$  of ATLAS data", *Phys. lett., Sect. B*, vol. 706, no. 2/3, pp. 150-167, 2011.
- 6. ATLAS Collaboration: G. Aad et al. (3027 authors), "Measurement of the jet fragmentation function and transverse profile in proton-proton collisions at a center-of-mass energy of 7 TeV with the ATLAS detector", The European physical journal. C, vol. 71, no. 11, pp. 1795-1-1795-25, 2011.
- 7. ATLAS Collaboration: G. Aad et al. (3030 authors), "Measurement of the transverse momentum distribution of  $Z/\gamma^*$  bosons in protonproton collisions at  $\sqrt{s} = 7$ TeV with the ATLAS detector", *Phys. lett.*, Sect. B, vol. 705, no. 5, pp. 415-434, 2011.
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- 12. ATLAS Collaboration: G. Aad et al. (3004 authors), "Search for massive colored scalars in four-jet final states in  $\sqrt{s} = 7$ TeV proton-proton collisions with the ATLAS detector", The European physical journal. C, vol. 71, no. 12, pp. 1828-1-1828-19, 2011.
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- 16. ATLAS Collaboration: G. Aad et al. (3026 authors), "Search for the Higgs boson in the  $H \rightarrow WW \rightarrow lvjj$  decay channel in pp Collisions at  $\sqrt{s} = 7$ TeV with the ATLAS detector", *Phys. rev. lett.*, vol. 107, no. 23, pp. 231801-1-231801-18, 2011.
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the ATLAS detector", *J. high energy phys.*, vol. 2011, no. 9, pp. 072-1-072-42, 2011.

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- 51. ATLAS Collaboration: G. Aad *et al.* (3064 authors), "Search for supersymmetry in *pp* collisions at  $\sqrt{s} = 7$ TeV in final states with missing transverse momentum and b-jets", *Phys. lett., Sect. B*, vol. 701, no. 4, pp. 398-416, 2011.
- 52. ATLAS Collaboration: G. Aad *et al.* (3050 authors), "Search for supersymmetry using final states with one lepton, jets, and missing transverse momentum with the ATLAS detector in  $\sqrt{s}$  = 7TeV *pp* collisions", *Phys. rev. lett.*, vol. 106, no. 13, pp. 131802-1-131802-19, 2011.
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- 56. DELPHI Collaboration: J. Abdallah *et al.* (340 authors), "A study of the b-quark fragmentation function with the DELPHI detector at LEP I and an averaged distribution obtained at the Z Pole", *The European physical journal. C*, vol. 71, no. 2, pp. 1557-1-1557-29, 2011.
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- 66. AUGER Collaboration: Anna Anzalone *et al.* (488 authors), "Removal of streaking artefact in the images of the Pierre Auger Observatory infrared cameras", In: 100 years of cosmic ray physics: from pioneering experiments to physics in space: proceedings of the Cosmic Ray International Seminars (CRIS 2010), Catania, Italy, *Nucl. Phys., B Proc. suppl.*, vol. 212/213, pp. 279-285, 2011.
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#### TEXTBOOKS AND LECTURE NOTES

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#### PH. D. THESIS

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# DEPARTMENT OF INORGANIC CHEMISTRY AND TECHNOLOGY K-1

The Department of Inorganic Chemistry and Technology is one of the leading groups in the world in the field of the synthesis of new inorganic compounds containing fluorine. 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 of colleges and elementary schools.



In the field of the research of new inorganic compounds containing fluorine, the research of coordination compounds with two perfluorinated anions was extended to the study of the parameters that affect the crystal structure and packing of perfluoro anions of different geometries in the unit cell. The set of compounds of the type  $[M(BF_{4})(AF_{6})]$  was extended on the calcium and cadmium metals. The following compounds were synthesized Head: and structurally characterized:  $[Ca(BF_4)(AF_4)]$  where A could be As, Sb, Bi, Ru, V, Nb, Ta and compounds of the Asst. Prof. Gašper Tavčar type  $[Cd(BF_4)(AF_4)]$ , where A is Ta and Bi. The compounds were prepared in two ways: with the dissolution of equimolar amounts of separately synthesized  $M(BF_{4})_{2}$  and  $M(AF_{4})_{2}$  in anhydrous HF or with an *in-situ* formed  $AF_{4}$ anion in anhydrous HF with the reaction between AF, and MF, in the mole ratio 2:1 followed by the addition of the corresponding amount of  $M(BF_4)_{a}$ . Both synthetic routes are equivalent. The calcium compounds are isostructural

with their strontium and barium analogues, while the structures of the cadmium compounds are different from the structures of so-far prepared compounds of the type  $M(BF_{4})(AF_{4})$ . During the synthesis of the compound  $Cd(BF_4)(VF_6)$ , two new compounds  $Cd(VF_6)_2$  and  $Cd(VOF_4)(VF_6)$  were obtained and their crystal structures were determined. The reactions of VOF,

with metal fluorides in a basic anhydrous HF were continued. A series of new compounds was isolated, e.g., the dimeric anion  $(V_2 O_2 F_8)^{2-}$ , as in  $[Pb(V_2 O_2 F_8)]$ ,  $[Ca(V_2 O_2 F_8)]$  and  $[Li_2(V_2 O_2 F_8)]$ ; the anion  $(V_3 O_3 F_{12})^{3-}$  present in the compound  $[Sr_3(HF)_6(V_3O_3F_{12})_2]$  and completely new anions  $(V_4O_3F_{18})^{5-}$ , found in the structure of the compound  $[Pb_{2}F(V_{4}O_{2}F_{10})]$  and  $(V_{2}O_{2}F_{2})^{-}$  found in the compound  $[Rb(V_{2}O_{2}F_{2})]$ .

The first compound with XeF, as a ligand was isolated as early as in 1991. In 2011, twenty years later, we succeeded in isolating the analogous krypton compound  $[Mg(KrF_2)_4(AsF_4)_2] \cdot 2BrF_5$  within a cooperation with the group of Prof. G. J. Schrobilgen from McMaster University in Canada. With this experiment it was also proven that the thermodynamically unstable KrF<sub>2</sub> could be used as a ligand to the metal ion.

The syntheses of the compounds of the type  $XeF_2 \cdot MF_4$  where M is Ti, Sn were continued in order to establish in which crystallographic types the compounds XeF<sub>2</sub>·MF<sub>4</sub> crystallize. The main purpose of this research was to finally solve the structure of the compound XeF<sub>2</sub>·PtF<sub>2</sub>, the first compound of the noble gas xenon, synthesized back in 1962. With Prof. S. H. Strauss from Colorado State University we cooperate in the field of compounds with the super weakly coordinating anion  $B_{12}F_{12}^{2-}$ . The compound  $[Ba(HF)_3(B_{12}F_{12})]$ was isolated and its structure was determined.

Reactions between different starting ratios of imidazole (Im;  $C_2H_2N_2$ ) and  $TiF_4$  in anhydrous HF yield  $[ImH]_2[TiF_4] \cdot 2HF$ ,  $[ImH]_2[TiF_{11}]$ ,  $[ImH]_4[Ti_4F_{20}]$ , [ImH]<sub>2</sub>[Ti<sub>4</sub>F<sub>22</sub>] and [ImH][Ti<sub>2</sub>F<sub>6</sub>]. In the crystal structure of [ImH]<sub>2</sub>[TiF<sub>6</sub>] 2HF, two HF molecules are found to be coordinated to the  $[TiF_c]^2$  anion by strong hydrogen bonds. The crystal structure of [ImH], [Ti,F<sub>11</sub>] consists of [ImH]<sup>+</sup> cations and  $[Ti_{1}F_{11}]^{3}$  anions. The  $[Ti_{2}F_{11}]^{3}$  dimer results from the association of two TiF<sub>6</sub> units by one corner. There are three crystallographically independent [Ti2F11] units with different geometries, orientations and different coordination with imidazolium cations. The tetrameric  $[Ti_4F_{20}]^{4-}$ 

Prof. Boris Žemva received a Zois Award for lifetime achievements in the field of inorganic fluorine chemistry



Figure 1: New anion  $(V_4 O_3 F_{18})^5$  determined in the structure of  $[Pb_{2}F(V_{4}O_{3}F_{18})].$ 

anion, found in the crystal structure of  $[ImH]_4[Ti_4F_{20}]$ , is made from four  $TiF_6$  octahedra sharing corners and forming, in that way, a square  $Ti_4F_{20}$  entity. The  $[ImH][Ti_4F_{20}]$  compound was found to crystallise in two different crystal modifications at ambient (298 K) and low (200 K) temperature. The crystal structure of  $[ImH]_3[Ti_5F_{23}]$  represents the first case where the pentameric  $[Ti_4F_{23}]^3$  anion built up from five octahedral  $[TiF_6]$  units has been observed.



Figure 2: Si(II) adduct with borane

Four TiF<sub>6</sub> octahedra share two neighbour apexes, forming a tetrameric ring. The fifth TiF<sub>6</sub> unit shares three apexes with three octahedra of the tetrameric ring. The [ImH][Ti<sub>2</sub>F<sub>9</sub>] also crystallizes in two different crystal modifications (low temperature, determined at 200 K and high temperature, determined at 298 K). It contains the polymeric  $([Ti_2F_9]^-)_n$  anion, which appears as double zig-zag chains made from TiF<sub>6</sub> units. The positive charge is balanced by the [ImH]<sup>\*</sup> cation.

Research of the properties of low-valent silicon compounds, where silicon is stabilized by large organic electron donor groups, was continued. The focus was set on three sylilenes: RSi (R= CH(C=CH<sub>2</sub>)(CMe)(2,6-*i*Pr<sub>2</sub>C<sub>6</sub>H<sub>3</sub>N)<sub>2</sub>), RSiCl<sub>2</sub> (R=1,3-bis(2,6-diizopropilfenil)imidazol-2-ylidene) and RSiCl (R=PhCN(*f*Bu)<sub>2</sub>). We have tested their reactivity with unsaturated compounds cyclooctatetraene, benzoil pyridine, diisopropyl azodicarboxylate and 1,2 diphenylhydrazine. In all cases a five-membered heterocyclic ring was formed through [1 + 4] cycloaddition. In contrast with the previous results, reactions

with carbodiimide led to the formation of silaimine, while the reaction with isocyanate led to the formation of fourmembered Si<sub>2</sub>O<sub>2</sub> rings. The adduct between the dichlorosylilenes RSiCl<sub>2</sub> (R=1,3-bis(2,6-diizopropilfenil)imidazol-2ylidene), RSiCl (R=PhCN(*t*Bu)<sub>2</sub>) and BH<sub>3</sub> was successfully prepared and characterized.

Using electrochemical synthesis, complexes of copper(I) chloride, bromide, nitrate, tetrafluoroborate, perchlorate, trifluoroacetate and trifluoromethylsulfonate with allyl derivatives of thiadiazoles and tetrazoles have \_\_\_\_\_\_ been obtained and structurally investigated.

Dr. Zoran Mazej together with the research group of Prof. Grochala from the University of Warsaw published an article in the journal Chemistry – A European Journal, 2011, 17, 10481 about the thermal decomposition of AgSO<sub>4</sub>, which was selected for the cover photograph. In cooperation with the Department of Physical and Organic Chemistry, hybrid compounds with  $ICl_2$  and  $IBr_2$  anions were structurally investigated.

In the research field of new materials with special properties the investigation of the structural and magnetic properties of the Ag(II) ternary fluorides should be mentioned. The research was done within a cooperation with Polish partners (University of Warsaw). Research in the

field of ferroelectric and ferroelectric fluoride materials was continued. Polaronic behaviour was discovered for the compound  $(NH_4)_3FeF_6$ , which is the first case where such behaviour was observed for a non-magnetoelectric fluoride. Research of heterogeneous reactions of trifluoromethane with some metal oxides, hydroxides, and carbonates at relatively low temperatures was continued. It was found that with alkali hydroxides complete decomposition (mineralisation) of stable trifluoromethane is achievable at temperatures that are approximately 1000 K lower



Figure 3: SEM image of an aerogel based on aluminium(III) fluoride; aerogel with composition  $AlF_{2,9}(OH)_{0,1}$ ,  $yH_2O$  is composed of anisotropic nanosized particles (30 nm x 300 nm) that are weakly interconnected and form a very open structure.

than those used in conventional processes of thermal decomposition. Aerogels based on aluminium(III) fluoride were prepared for the first time by supercritical drying of the corresponding fluoride sols or gels in alcoholic media. The exceptional voluminosity of these materials is the result of the formation of anisotropic nanosized particles that are weakly interconnected forming very open structures. In cooperation with the Sts. Cyril and Methodius University in Skopje the quantum chemical modelling of some adsorption processes that enable the additional characterisation of the solid surfaces of adsorbents or catalysts were continued. The modelling of pyridine adsorption on aluminium(III) oxide or on partially fluorinated aluminium(III) oxide showed that the gradual replacement of oxide ions with fluoride ions increases the acidity of these materials, which is in accordance with qualitative experimental findings.

In the framework of a cooperation with the Centre of Excellence PoliMaT, new hydrophilic aromatic hydrocarbon plasma polymers with incorporated amino functional groups were prepared and characterized. The antimicrobial activity of these kinds of polymers suggests possible applications as coatings in medicine. From coordination compounds, transition-metal sulphides were prepared, which are interesting for catalytic applications in gas-phase reactions due to their high specific surface area. The activity of the tested appropriate transition-metal oxides scored even higher. Research was conducted in cooperation with the Centre of Excellence NANOCENTER.

The next major activity of the group has been devoted to technological, ecological and safety problems. In the past year different plants used for the preparation of herbal tea infusions were tested for the purpose of monitoring environmental pollution with fluorine. The degree of fluorine pollution in the vicinity of fluorine-emitting plants can be correlated mostly with the content of free fluoride in the soil. Less but still important factors are the total fluorine in the soil, the pH of the soil and the wind direction. In the area of electrochemistry, new methods applicable

to the calibration of indicator electrodes were suggested. In the analytical laboratory the new elemental analyser Elementar, vario EL cube suitable for a determination of the CHNS composition was installed and put into full operation. The research on the transformation of contaminated biomass to clean fuels was finished and the research on the optimisation of the final solution of PCB-contaminated landfill continued. We also proceeded with the work in the project Access to Technology and Know-How in Cleaner Production in Central Europe (Act Clean). The research on the optimisation

With alkali hydroxides the complete decomposition (mineralisation) of stable trifluoromethane is achievable at temperatures that are approximately 1000 K lower than those used in the conventional processes of thermal decomposition.

of 3d dispersion field in a wet scrubber in a pilot plant with a capacity of  $1,200 \text{ m}^3$  was continued. The experimental data are being processed.

We started 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. It deals with the continuation of the research of the chemistry of catalytic oxidation of mercury in wet flue gas desulphurisation processes. The partners in the 3-year project are the departments O2, K1 and the Faculty of Chemistry and Chemical Technology of the University of Maribor. The process attracted quite an interest in professional community and for this reason, prof. dr. Xiang Gao from State Key Laboratory for Clean Energy Use, Institute for Thermal Power Engineering, Zhejiang University, Hanzhou, PR China applied at the Chinese research agency for funds for a Chinese-Slovenian bilateral cooperation on this theme. In the scope of Chinese-Slovenian cooperation in the field of environmental protection technologies a second workshop entitled "Development of

processes and equipment for flue gas purification" took place at the Institute from 9 to 11 November 2011. The workshop ended with an agreement on a continuation of the cooperation in the following areas: development of catalytic oxidation of mercury in wet FGD processes, the application of our model for the optimisation of chemistry and hydrodynamics of the wet scrubber, training of Chinese students in the IPS at the JSI and of our students in Zhejianf Unversity, training of Chinese doctor candidates in mercury analytics in the department O2.

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 five (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 2011, when Ljubljana city centre was closed to private motorised traffic.



Figure 4: Laboratory experiment on the influence of fluorine on the development of plants, preparation of the samples (nettles).

In the EU FP7 project Integ-Risk we continued our work on the key *development of plants, preparation of* performance indicators on the quality for mutual consideration of the process safety risk assessment and spatial planning process. In addition, we worked on a proposed approach integrating risk assessment for emerging risks into the environmental impact assessment procedures (considering levels from strategic down to the project/technology).

In the field of process safety (industrial risks) we have been engaged in consultations with local industry. With the Thermal power plant Brestanica d.o.o. we have provided consultation services related to the implementation of a safety-management system, risk assessment and the preparation of the related report for the licensing procedure (in the context of EU directive 96/82/EC, or Seveso II).

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. A part of these activities is included in the European project KidsINNscience. New methods for learning natural sciences were tested. With demonstrations of

chemical experiments we participated at the 17<sup>th</sup> Slovenian Science Festival, organized by the Slovenian Science Foundation, at the 4th 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 2011

- 1. Shabana K., Sen S. S., Kratzert D., Tavčar G., Roesky H. W., Stalke D., Synthesis of stable silicon heterocycles by reaction of organic substrates with a chlorosilylene [PhC(NtBu),SiCl]. Chemistry (Weinh., Print). 17 (2011), 4283-4290
- 2. Malinowski P., Derzsi M., Budzianowski A., Lesczzyński P. J., Gawel B., Mazej Z., Grochala W., Unusual thermal decomposition of Ag(II)SO<sub>4</sub> yielding Ag<sub>2</sub>(I)S<sub>2</sub>O<sub>5</sub> : bending Hammond's rule. Chemistry (Weinh., Print), 17 (2011) 10324-10327
- Radan K., Lozinšek M., Goreshnik E. A., Žemva, B., Syntheses, structures and Raman spectra of  $Cd(BF_4)(AF_4)$ 3. (A = Ta, Bi). J. Fluorine Chem., 132 (2011) 767-771
- Nastova I., Skapin T., Pejov, L., Effect of partial fluorination on the Lewis sites of microcrystalline [gamma]alumina studied by adsorption of pyridine as a probe molecule : a quantum chemical cluster model study. Surf. Sci., 605 (2011) 1525-1533
- 5. Koblar A., Tavčar G., Ponikvar-Svet M., Effects of airborne fluoride on soil and vegetation. J. Fluorine Chem., 132 (2011) 755-759

#### Patents granted

- Procedure for synthesis of threadlike tungsten oxide W5014 1. Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih EP2114827 (B1), European Patent Office, 16.2.2011.
- Process for the synthesis of nanotubes and fullerene-like nanostructures of transition metal dichalcoge-2. nides, quasi one-dimensional structures of transition metals and oxides of transition metals Aleš Mrzel, Maja Remškar, Adolf Jesih, Marko Viršek US8007756 (B2), United States Patent and Trademark Office, 30.8.2011.

#### Awards and appointments

Prof. Boris Žemva: Zois's award for lifetime work on the field of inorganic fluorine chemistry. 1.

## INTERNATIONAL PROJECTS

- 1. Innovation in Science Education Turning Kids on to Science KidsINNscience
  - 7. FP, 244265

EC; Nadia Prauhart, Markus Meissner, Austrian Institute of Ecology, Vienna, Austria Tomaž Ogrin, M. Sc., Dr. Špela Stres

- 2. Early Recognition, Monitoring and Integrated Management of Emerging, New Technology Related Risks
  - iNTeg-Risk
  - 7. FP, 213345, NMP2-LA-2008-213345

EC; European Virtual Institute for Integrated Risk Management, Stuttgart, Germany Asst. Prof. Marko Gerbec, Prof. Branko Kontić 3

- Mobilising Citizens for Vital Cities Ljubljana-Gent-Zagreb-Brno-Porto
- CIVITAS-ELAN
- 7. FP, 218954, TREN/FP7TR/218954
- EC; Zdenka Šimonovič, Mestna občina Ljubljana, Ljubljana, Slovenia
- Asst. Prof. Marko Gerbec, Dr. Davor Kontić, Prof. Branko Kontić Access to Technology and Know-how in Cleaner Production in Central Europe 4 ACT CLEAN
  - Central Europe Programme

EC; Jakob Gross, Horst Pohle, Federal Environment Agency, Dessau-Roßlau, Germany Dr. Andrej Stergaršek, Tanja Zdolšek, Andrej Gyergyek, B. Sc., Asst. Prof. Sonja Lojen

- 5 Evaluation, Improvement and Guidance for the Use of Local-scale Emergency Prediction and Response Tools for Airborne Hazards in Built Environments COST ES1006
  - EC; COST Office, Brussels, Belgium
  - Asst. Prof. Marko Gerbeo
- Novel Flurides of Divalent Silver and Palladium: Various Pathways Towards 6 Superconductivity
  - BI-PL/10-11-003

Dr. Grochala Wojceich, The University of Warsaw, Warsaw, Poland Dr. Zoran Maze

Tungsten Carbide: Fine Powders Obtaining and Coatings Deposition from Melts,

Regeneration from Industrial Wastes

BI-UA/11-12-009

Dr. Igor Astrelin, Faculty of Chemistry & Technology, National Technical University of Ukraine, "Kyiv Politechnic Institute", Kyiv, Ukraine Dr. Melita Tramšek

Selective Synthesis of Fulerenic Superhalogens and Flurinated Superweak Anions BI-US/11-12-030

Prof. Steven H. Strauss, Colorado State University, Department of Chemistry, Fort Collins, CO, USA Prof. Boris Žemvai

## R & D GRANTS AND CONTRACTS

- Speciation and interactions of chemical contaminants at trace level in aqueous media 1. to support the developement of cost-effective removal technologies Prof. Milena Horvat
- 2 Optimisation of a polychlorinated biphenyls' (PCBs) contaminated material dump site remediation Dr. Andrej Stergaršek
- The faith and speciation of pollutants in the transformation of contaminated biomass 3. into synthetic fuel and pure hydrogen Dr. Andrej Stergaršek

## RESEARCH PROGRAM

Inorganic chemistry and technology 1. Prof. Boris Žemva

### NEW CONTRACTS

1. Update of the threat assessment and operators security plans Geoplin Plinovodi d. o. o. Asst. Prof. Marko Gerbec

## VISITORS FROM ABROAD

- 1. Prof. dr. Gary J. Scrobilgen, McMaster University, Canada, 10-19. 9. 2011
- Prof. dr. Victor Malyshev and Tetiana Lukashenko, Faculty of Chemistry and
- Technology, National Technical University of Ukraine, Ukraine, 24-27. 10. 2011

2. Preparation of Environmental risk reduction plan Thermal Power Plant Brestanica Asst, Prof. Marko Gerbec

15. Igor Shlyapnikov

17. Aleš Štefančič, B. Sc.

18. Andrii Vakulka, M. Sc.

16. Matej Sedlar'

19. Gleb Vervasov

**Technical officers** 

20. Peter Frkal, B. Sc.

21. Tine Oblak, M. Sc.

23. Pero Kolobarić

25. Mira Zupančič

Note:

24. Robert Moravec

22. Tomaž Ogrin, M. Sc.

Technical and administrative staff

\*\* postgraduate financed by industry

- Dr. Angelina Gab and dr. Dmytro Shakhinin, National technical University of Ukraine, Ukrajine, 24-31. 10. 2011
- 4. Dr. Weng Weiguo and co-workers, Zhejiang University LCEU, Hangzhou, 9-11. 11. 2012

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- Asst. Prof. Marko Gerbec 1.
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- Dr. Adolf Jesih 3.
- Asst. Prof. Robert Kocjančič 4.
- Dr. Zoran Mazei 5
- Asst. Prof. Maja Ponikvar-Svet 6.
- Asst. Prof. Tomaž Skapin
- 8 Dr. Andrej Stergaršek
- 9. Asst. Prof. Gašper Tavčar, Head
- 10. Dr. Melita Tramšek

#### 11. Prof. Boris Žemva Postgraduates

- 12. Alenka Koblar, B. Sc. 13. Matic Lozinšek, B. Sc.
- 14. Kristian Radan, B. Sc.

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- 2. Ramachandran Azhakar, Sankaranaraya Pillai Sarish, Gašper Tavčar, Herbert W. Roesky, Jakob Hey, Dietmar Stalke, Debasis Koley, "Formation of silicon centered spirocyclic compounds: reaction of Nheterocyclic stable silylene with benzoylpyridine, diisopropyl azodicarboxylate, and 1,2-diphenylhydrazine", Inorg. chem., vol. 50, no. 7, pp. 3028-3036, 2011.
- 3. Ramachandran Azhakar, Gašper Tavčar, Herbert W. Roesky, Jakob Hey, Dietmar Stalke, "Facile synthesis of a rare chlorosilylene-BH<sub>3</sub> adduct", European Journal of Inorganic Chemistry, vol. 2011, no. 4, pp. 475-477, 2011.
- 4. Mariana Derzsi, Przemyslaw Malinowski, Zoran Mazej, Wojciech Grochala, "Phonon spectra and phonon-dependent properties of AgSO<sub>4</sub>, an unusual sulfate of divalent silver", Vibr. spectrosc., vol. 57, no. 2, pp. 334-337, 2011.
- 5. Cene Filipič, Vid Bobnar, Gašper Tavčar, Boris Žemva, Adrijan Levstik, "Polarons in low temperature phase of (NH<sub>4</sub>)<sub>3</sub>FeF<sub>6</sub>", J. appl. phys., vol. 110, no. 9, pp. 093721-1-093721-3, 2011.
- 6. Evgeny A. Goreshnik, Vladimir Gelmboldt, Larisa Koroeva, Eduard Ganin, "Synthesis, crystal structure and properties of 3-5-diamino-1,2, 3-triazolium (LH) salts (LH)<sub>2</sub>SiF<sub>6</sub>, (LH)BF<sub>4</sub> and [Cu(LH)<sub>2</sub>]<sub>2</sub>(siF<sub>6</sub>)<sub>3</sub>", J. fluorine chem., vol. 132, issue 2, pp. 138-142, 2011.
- 7. Evgeny A. Goreshnik, Marian G. Mys'kiv, "Synthesis and crystal structure of copper(I) nitrate  $\pi$ -complex with 1-allylbenzotriazole of equimolar composition", Acta chim. slov., vol. 58, no. 4, pp. 772-775, 2011.

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- 12. Przemysław Malinowski, Zoran Mazej, Mariana Derzsi, Zvonko Jagličić, Jadwiga Szydłowska, Tomasz Gilewski, Wojciech Grochala, "Silver(II) triflate with one-dimensional  $[Ag(II)(SO_3CF_3)_{4/2}] \infty$  chains hosting antiferromagnetism", CrystEngComm (Camb., Online), vol. 13, no. 22, pp. 6871-6879, 2011.
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#### REVIEW ARTICLES AND CHAPTERS IN BOOKS

- 1. Maja Ponikvar-Svet, Joel F. Liebman, "Interplay of thermochemistry and Structural Chemistry, the journal (volume 21, 2010) and the discipline", *Struct. chem.*, vol. 22, no. 3, pp. 717-740, 2011.
- 2. Maja Ponikvar-Svet, Joel F. Liebman, "Interplay of thermochemistry and Structural chemistry, the journal (volume 22, 2011, issues 1-3) and the discipline", *Struct. chem.*, vol. 22, no. 3, pp. 717-740, 2011.

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#### Regular papers

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- 3. Tine Oblak, Tina Oblak, Jože Oblak, "Smrekova smola, njeni blagodejni učinki ter uporaba nekoč in danes", In: *Zbornik referatov*, 24. seminar Poslovno proizvodni trendi, razviti svet in mi in tirideseto srečanje strojnikov 64', Krško, 24. in 25. november 2011, Tadej Jakopič, ed., Ljubljana, Društvo Machinatores, 2011, pp. 99-104.
- 4. Zdenka Peršin, Karin Stana-Kleinschek, Adolf Jesih, Uroš Maver, "Plasma - assisted surface modification of poly(ethyleneterephtalate) for antimicrobial wound-dessing", In: *Conference proceedings*, 4th International Conference on Advanced Plasma Technologies (iCAPT-IV) with Workshop on Plasma Synthesis and Applications of Nanomaterials & 112th IUVSTA Executive Council Meeting, September

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- 7. Igor Shlyapnikov, Evgeny A. Goreshnik, Zoran Mazej, "Poly[perfluorotitanate(VI)] compounds, Synthesis, characterization, application", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 54-59.
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- Andrii Vakulka, Tomaž Škapin, "Acid-Base nature of the reaction between trifluoromethane and different hydroxides and carbonates", In: *Slovenski kemijski dnevi 2011, Portorož, 14-16 september 2011,* Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2011, 7 pp.

#### TEXTBOOKS AND LECTURE NOTES

- 1. Ester Heath, Tina Kosjek, Jernej Iskra, David Heath, Tomaž Skapin, *Extraction techniques for the green chemist: učno gradivo pri predmetu "Green Chemistry"*, Ljubljana, Jožef Stefan International Postgraduate School, 2011.
- 2. Ester Heath, Tina Kosjek, Jernej Iskra, David Heath, Tomaž Skapin, Extraction techniques for the green chemist: učno gradivo pri predmetu "Tools for the environmental quality control - organic pollutant in the environment", Ljubljana, Jožef Stefan International Postgraduate School, 2011.

#### B. SC. THESIS

1. Aleš Štefančič, Synthesis and characterization of aerogels based on aluminium(III) fluoride: undergraduate thesis, Ljubljana, [A. Štefančič], 2011.

#### PATENTS

- 1. Aleš Mrzel, Maja Remškar, Adolf Jesih, Marko Viršek, Process for the synthesis of nanotubes and fullerene-like nanostructures of transition metal dichalcogenides, quasi one-dimensional structures of transition metals and oxides of transition metals, US8007756 (B2), United States Patent and Trademark Office, 30.8.2011.
- 2. Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih, *Procedure for synthesis of threadlike tungsten oxide W*<sub>5</sub>*O*<sub>14</sub>, EP2114827 (B1), European Patent Office, 16.2.2011.

#### PATENT APPLICATION

1. Adolf Jesih, Andrej Kovič, Aleš Mrzel, *Procedure for the synthesis of quasi one-dimensional structures of 4d and 5d (Nb, Mo, Ta, W) transition metals*, P-201100223, Urad RS za intelektualno lastnino, 24.6.2011.

## 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 halogenated, in particular fluorinated, organic molecules.

**Experimental research in the field of electrochemistry** continues for the materials that are important in biomedical and technological applications. Corrosion protection of the allovs used in these applications can be achieved by various treatments - from surface layers to functional modifications of the surface and corrosion inhibitors. In our work we focus on all these modes of protection. The formation of surface layers, usually oxides, is an effective way of passivating the underlying metal substrate. In 2011 we were devoted to the protection of Nitinol. Nitinol is the commercial name for an alloy containing nearly equi-atomic composition of nickel and titanium. This alloy was developed in the 1970s and was very soon explored for biomedical purposes, first in orthodontic treatments, and later in cardiovascular surgery for stents and guide wires, in orthopaedic surgery for various staples and rods, and in maxillofacial and reconstructive surgery. A Nitinol alloy exhibits two closely related and unique properties: Head: shape memory and superelasticity. Although Nitinol contains 50 at.% of titanium, its corrosion properties are inferior Prof. Ingrid Milošev to this metal. Under certain conditions in a simulated physiological solution it is subjected to the localized-corrosion phenomenon. In order to increase its corrosion protection we have explored several treatments. Surface preparation



- grinding or polishing - is shown to have a decisive role in improving the corrosion properties with surface treatments. Low-temperature treatments like boiling in water and thermal oxidation at 100 °C resulted in the formation of oxide layers only a few nanometres thick, composed mainly of TiO<sub>2</sub> and a small amount of NiO. These layers are well able to protect the underlying Nitinol substrate. Up to 500 °C, surface preparation directly determines the thickness of the oxide scale, as a 20-fold difference in thickness is observed between the ground and the polished samples. At higher temperatures, the oxide thickness was similar for the two samples. A multilayer structure is observed at all the temperatures investigated. The outermost layer at the oxide/air interface is composed of TiO<sub>2</sub> and NiO, while the interior of the oxide scale is composed exclusively of TiO2. The oxide layers formed with thermal oxidation at elevated temperatures also improve the corrosion characteristics of Nitinol, especially for polished substrates. Important information in terms of biocompatibility is that the content of nickel in the oxide layer is very low. As nickel is a known allergen, its dissolution in human body should be as low as possible. Therefore, the treatments used for increasing the corrosion protection are also beneficial for biocompatibility.

The formation of various coatings on the surface of metals and alloys is another way of corrosion protection of technologically important materials like aluminium and its alloys. In the past these materials were protected by using conversion chromate coatings. Because of cancerogenicity and toxicity of the chemicals used in their production, the use of chromate coatings has been banned. In the last decade numerous studies were devoted to the investigations of alternative ways of protecting aluminium alloys. One of the possibilities is silane coating, which represents a non-toxic, environmentally friendly replacement for coatings with hexavalent chromium. In collaboration with a group from the Faculty of Technology and Metallurgy, Belgrade, we studied vinyltriethoxysilane coatings on aluminium. Using X-ray photoelectron spectroscopy we identified Si-O-Si and Si-O-Al bonds and thus contributed to the clarification of the formation mechanism for the silane coatings on aluminium and the mechanism of their corrosion protection. In our laboratory we started the synthesis of the hybrid sol-gel coatings using a spin coater for protecting aluminium and its alloys (AA2024



Figure 1: (a) SEM image of a Nitinol surface prepared by polishing and then subjected to a thermal oxidation at 500°C showing grains of an oxide product. Magnification 10,000× (b) Potentiodynamic polarization curves recorded in a simulated physiological solution for polished Nitinol, and Nitinol oxidized for 1 h at various temperatures, dE/dt=1mV/s.

Oxide layers formed with thermal oxidation at low and elevated temperatures improve the corrosion characteristics of Nitinol. This treatment, used for increasing the corrosion protection, is also beneficial for biocompatibility, as the content of nickel in the oxide layer is very low. and AA7075). The process of coating deposition is optimized using in-situ FT-IR AR spectroscopy. Deposited coatings are then characterized using electrochemical methods, the salt spray testing, as well as the methods for morphological and surface characterization.

Functional modifications of the surface can be performed using a self-assembling procedure. In collaboration with the Faculty of Chemical Engineering and Technology from the University of Zagreb we investigated the possibility to change the interface structure and the surface chemistry of the Nitinol surface with the octadecylphosphonic acid. As a result, a self-

assembled, covalently bonded (a monodentate type) film was formed. We investigated the structure and composition of the films formed with two different deposition methods.

The precise atomic-scale mechanism of the functioning of corrosion inhibitors is usually not known, yet it is



Figure 2: Crevice and fretting corrosion in the interior between a femoral neck made of the Ti-6Al-4V alloy and a femoral head made of stainless steel. The prosthesis was revised due to aseptic loosening after 12 years in situ. (a) The femoral stem and the femoral head cut in half. Fretting scars at the neck are denoted by short arrows, (b) SEM image of fretting scars, (c) SEM image of a corrosion product formed in the interior of the femoral head, and (d) an EDS spectrum of the corrosion product presented in (c). generally accepted that, in the majority of cases, the inhibition of corrosion is achieved through the interaction between the corrosion-inhibitor molecules and the surface of the metal. For this reason we investigated, by means of first-principles density-functional theory (DFT) based on computer simulations, how the azole-based corrosion inhibitors-such as imidazole, triazole, benzotriazole, naphthotriazole, and tetrazole-interact with copper and aluminum surfaces. We found that the chemistry of azoletype inhibitors is very diverse on the surfaces of metals. These molecules can adsorb in different forms or even associate in various intermolecular aggregates, such as organometallic complexes. Several of the considered azole molecules can chemisorb perpendicularly to the surface or physisorb with the molecular plane being nearly parallel to the surface. While the magnitude of the chemisorption energy increases as passing from densely packed Cu(111) to more open surfaces and low coordinated surface defects. the physisorption energy is much less sensitive to surface details. We also found that, in general, deprotonated inhibitor molecules interact far stronger with metal surfaces than with neutral molecules, and with the help of the solvation effects they are able to replace reactive corrosive species, such as chloride, from the surface of a metal, thus reducing the rate of corrosion. These DFT computer simulations have thus provided many details about the interaction of the azole inhibitor molecules with the copper surfaces, which is now better understood at the atomic level.

Our studies on biomedically important materials, which have been in progress for more than ten years, cover different fields. Our collaboration with the groups from the Institute "Ilie Murgulescu" from Bucharest and the University of Primorska is devoted to a new alloy containing titanium, niobium and zirconium. The alloy is based on the nano-architecture bioalloy/ nanometre oxide layer/nanometre functional layer. We are interested in the electrochemical behaviour of this material under simulated physiological

conditions and its cytotoxicity. Our long-term collaboration with the Valdoltra Orthopaedic Hospital continues to be devoted to the effects of various physiological conditions on the corrosion stability of the three most important groups of orthopaedic materials. The combination of corrosion and wear of the joint replacements often leads to

First-principles density-functional theory based on computer simulations provided us with many details about the interaction of azole corrosion inhibitor molecules with the copper surfaces that is now better understood at the atomic level.

both crevice and fretting corrosion. Corrosion products containing iron and chromium oxides were identified in the components made of stainless steel. Fretting corrosion is a form of damage occurring at the interface of two closely fitted surfaces, when they are subjected to a slight oscillatory slip and to joint corrosion actions. Crevice corrosion is a type of localized corrosion closely related to pitting corrosion. It occurs primarily in the regions of a metal surface, where mass transfer is limited, e.g., in narrow crevices or

under deposits. On these occluded areas, the concentration of aggressive chloride ions, a decrease in the pH value, and the depletion of oxygen can rapidly lead to surface activation.

**Our theoretical investigations** of the atmospherically relevant radical reactions were based on the quantum chemical methods and continued to examine the mechanism of the reaction of the sulphur-containing radicals with  $NO_x$ . The overall mechanism for the HOSO +  $NO_2$  singlet radical-radical reaction can be summarized

as an initial association of radicals, followed by isomerization and/or dissociation of intermediates. The direct hydrogen-abstraction mechanism is less likely to occur.

Further, the peroxy-nitrite association adducts, CH<sub>2</sub>XCH<sub>2</sub>OONO, and the isomeric nitrate compounds, CH<sub>2</sub>XCH<sub>2</sub>ONO<sub>2</sub> (X=O,S), in the reaction of NO with CH<sub>2</sub>XCH<sub>2</sub>O<sub>2</sub> are characterized computationally and the heat-offormation parameters are evaluated. The dissociation channels into the alkoxy radicals and nitrogen dioxide, CH<sub>3</sub>XCH<sub>2</sub>O+NO<sub>2</sub>, are examined in detail Figure 3: Reaction scheme for HOSO + NO<sub>2</sub> and are found to proceed via low activation barriers, located late in the exit

valley. The small energy difference, determined between the activation barriers in favour of the sulphuric system, is suggested to be the main factor that differentiates the reactivity of the two homologous reactions, CH<sub>2</sub>OCH<sub>2</sub>O<sub>2</sub>+NO and CH<sub>2</sub>SCH<sub>2</sub>O<sub>2</sub>+NO, and explains the larger rate constant measured experimentally for the latter system.

In the framework of the Laboratory for Organic and Bioorganic Chemistry we continued the investigation of the application of the principles of green chemistry in the transformations of organic compounds stressing the selective introduction of halogen atoms into organic compounds. We discovered and developed a new method for aerobic oxidative halogenations of organic compounds, based on the catalytic cycle of nitrogen oxides, derived from the acid-supported and thermally accelerated transformations of nitrate anion, while molecular

iodine or bromide and chloride anions were used as sources of halogen atoms. We have preliminarily shown that this method could be used for an efficient iodination and bromination of organic compounds, while special attention was devoted to the optimization of the reaction parameters for the chlorination issue, still representing a considerable challenge in the framework of organohalogen chemistry. We discovered that the presence of catalytic amounts of molecular iodine is essential for the selective and efficient chlorination of a variety of ketones with air/NO<sub>3 (cat</sub>/HCl reaction system resulting in the selective and efficient formation of alpha-chloro substituted ketones. We have also improved the catalytic reaction system for the aerobic oxidative iodination of organic compounds air/HNO<sub>2</sub>(cat)/I<sub>2</sub> with a discovery that the turnover number of the process could be enlarged by a decade (from 5 to 50) with an addition of 5 mol % of H<sub>2</sub>SO<sub>2</sub> to the reaction system. On the basis of an invitation by the editorial board of the Molecules journal we prepared a review article entitled Recent Advances in the Application of Selectfluor F-TEDA-BF, as a Versatile Mediator or Catalyst in Organic Synthesis and published it in a special issue of the journal dedicated to fluoroorganic chemistry. The publication was already cited in Science. We are continuing our research on a selective synthesis of organic peroxides stressing transformations of ketones or aldehydes to dihydroperoxides known as precursors for a preparation of cyclic peroxides.

For the company Ecot we developed, constructed and tested an instrument for determining the freezing points of the liquid mixtures of ethanol/ water. The instrument serves as a control check point for the quality of producing the anti-freeze liquids for the car glass superficies. In the framework



Etheric and sulphuric nitrate isomers CH<sub>3</sub>XCH<sub>2</sub>ONO<sub>2</sub>, X=O,S are found to be significantly more stable than the peroxy nitrite isomers and may serve as reservoir compounds of methoxymethyl peroxy and methylthiomethyl peroxy radicals in the troposphere.





Figure 4: Homebuilt supercomputer named PARS consisting of 330 CPU cores (Intel Xeon and AMD Opteron) and 1080 GB of RAM and running on Debian GNU/Linux operating system

of the Centre of Excellence CIPKeBiP and in collaboration with the high-tech company ACIES BIO, we collaborated in a directed synthesis of potential bioactive compounds. We also collaborated with the company Semenarna on a synthesis of gamethocidic active compounds used in the production of plant hybrids.

#### Some outstanding publications in the last year

- 1. I. Milošev, Metallic Materials for Biomedical Applications: Laboratory and Clinical Studies, Pure Appl. Chem., 83 (2011), 309-324.
- 2. N. Kovačević, A. Kokalj, Analysis of Molecular Electronic Structure of Imidazole- and Benzimidazole-Based Inhibitors: A Simple Recipe for Qualitative Estimation of Chemical Hardness, Corrosion Sci., 53(2011), 909-921.

We discovered and developed a new method for the aerobic oxidative chlorination of organic carbonyl compounds, based on the catalytic cycle of nitrogen oxides, derived from acid-supported and thermally accelerated transformations of nitrate anion, while a chloride anion was used as the source of chlorine atoms.



Figure 5: Method for aerobic oxidative chlorination of ketones

#### Awards and appointments

- A. Kokalj, N. Kovačević, S. Peljhan, M. Finšgar, A. Lesar, I. Milošev, Triazole, Benzotriazole, and Naphthotriazole as Copper Corrosion Inhibitors: I. Molecular Electronic and Adsorption Properties, ChemPhysChem, 12 (2011), 3547–3555
- 4. A. Lesar and A. Tavčar, Atmospheric Reaction of the HOSO Radical with NO<sub>2</sub>: A Theoretical Study , J. Chem. Phys. A, 115 (2011), 11008-11015
- 5. S. Stavber, Recent Advances in the Application of Selectfluor F-TEDA-BF $_4$  as a Versatile Mediator or Catalyst in Organic Synthesis. Molecules 16 (2011), 6432-6464
- Ingrid Milošev: Zois Certificate of Recognition for significant achievements in the research of biocompatible materials and experimental orthopaedics in 2011
- Ingrid Milošev: Medal for exceptional contribution to the increase of reputation and recognition of the Valdoltra Orthopaedic Hospital in 2011

## INTERNATIONAL PROJECTS

- 1. Controlled Surface Structuring and Surface Functionalisation of Advanced Biomedical Titanium Alloys for Ortopaedic Implants
  - SURFUNCTI
  - MNT ERA NET II
  - 3211-10-000029
  - Institute of Physical Chemistry »Illie Murgulescu«, Bucharest, Romania Prof. Ingrid Milošev
- 2. Bioengineering Advanced Metallic Materials and Functional Coatings for Medical Application
  - BÎ-HR/10-11-015

Prof. Zoran Grubač, Kemijsko-tehnološki fakultet Sveučilišta u Splitu, Split, Croatia Prof. Ingrid Milošev

 Atomistic Computer Simulations of N<sub>2</sub>O Dissociation on Rh(100) and Rh(110) Surfaces and the Role of Coadsorbed Oxygen BI-IP/11-13-005

Dr. Orita Hideo, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan Dr. Anton Kokalj

4. Testing CIs for Metals in Different Media, with Emphasis on Acidic Media and Methane Sulfonic Acid (MSA)

Contract dtd. 24. 12. 2010

Dr. Fabio Nicolini, E-EMV/FM Metal Surface Treatment, BASF SE, Ludwigshafen/Rhein, Germany Dr. Matice Firstoar, Brof, Inggid Milosov

Dr. Matjaž Finšgar, Prof. Ingrid Milošev
 Reactions of S-Containing Radicals with Amines and NO<sub>x</sub>: A Theoretical Study BI-NO/11-12-010

Prof. Claus Jørgen Nielsen, University of Oslo, CTCC, Department of Chemistry, Oslo, Norway

Dr. Antonija Lesar 6. Electrochemical non-Metalic Coatings on Modified Metal Surfaces BI-SR/10-11-008

Prof. Vesna Mišković-Stanković, Faculty of Technology and Metallurgy, University of

## VISITORS FROM ABROAD

- Diana Blejan, B.Sc., University Babes-Bolyai, Cluj-Napoca, Romunia, 3 May 31 July 2011
   Dr. Monica Popa, Dr. Jose Calderon Moreno, Dr. Ecaterina Vascilescu, Dr. Corina
- Dr. Monica Popa, Dr. Jose Calderón Moreno, Dr. Ecaternia Vascilescu, Dr. Cornia Vascilescu, Institute of Physical Chemistry "Ilie Murgulescu", Bukarest, Romunia, 18 August 2011
   Dr. f. d. March Learne Leatistica of Diamedical Paralecence of Macanenastic
- Prof. dr. Marek Langer, Institute of Biomedical Engineering and Measurements, Wroclaw Technical University, Poland, 29 August 2011

Belgrade, Belgrade, Serbia Prof. Ingrid Milošev

## R & D GRANTS AND CONTRACTS

- 1. Role of molecular structure of inhibitors and their selfassembling in corrosion protection of metal surfaces
- Dr. Anton Kokalj 2. 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 polyoxometalates and TiO2 nanostrucutres for production of hydrogen by catalytic oxidation of water -NANOleaf Dr. Polona Umek
- Survivorship of total hip replacements as a function of type of bearing surfaces Prof. Ingrid Milošev

## RESEARCH PROGRAMS

- Multiphase nanoarchitectures: development, physical and chemical characterization and simulation of processes Prof. Ingrid Milošev
- Bioanorganic and bioorganic chemistry Prof. Stojan Stavber
- Laura Caselas Comelles, student of Faculty of Pharmacy, University of Barcelona, Spain, 27 September 2011 – 15 January 2012
- 5. Zoi Salta, B.Sc., University of Ioannina, Greece, 7-18 November 2011
- Prof. dr. Vesna Mišković Stanković, Faculty of Technology and Metallurgy, University of Belgrade, Serbia, 5–7 November 2011

### 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
- 6. Dr. Matjaž Finšgar
- Postgraduates
- 7. Leon Bedrač, B. Sc.

## BIBLIOGRAPHY

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- 1. Matjaž Finšgar, Ingrid Milošev, "Corrosion study of copper in the presence of benzotriazole and its hydroxy derivative", *Mater. corros.* (1995), vol. 62, issue 10, pp. 956-966, 2011.
- 2. Jernej Iskra, "Antimalarial peroxides: from artemisinin to synthetic peroxides", *J. malar. res.*, vol. 1, no. 1/2, pp. 1-40, 2011.
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- Darja Kek-Merl, Ingrid Milošev, Peter Panjan, Franc Zupanič, "Morphology and corrosion properties PVD Cr-N coatings deposited on aluminium alloys", *Mater. tehnol.*, vol. 45, no. 6, pp. 593-597, 2011.
- 6. Anton Kokalj, "Electrostatic model for treating long-range lateral interactions between polar molecules adsorbed on metal surfaces", *Phys. rev., B, Condens. matter mater. phys.*, vol. 84, no. 4, pp. 045418-1-045418-17, 2011.
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- Anton Kokalj, Nataša Kovačević, Sebastijan Peljhan, Matjaž Finšgar, Antonija Lesar, Ingrid Milošev, "Triazole, benzotriazole, and naphthotriazole as copper corrosion inhibitors. I., Molecular electronic and adsorption properties", *ChemPhysChem*, vol. 12, no. 18, pp. 3547-3555, 2011.
- 9. Agnie M. Kosmas, Stavroula Liaska, Antonija Lesar, "Theoretical characterization of the reactions  $CH_3XCH_2O_2 + NO$  (X = 0, S)", *J. mol. struct., Theochem*, vol. 967, no. 1, pp. 37-43, 2011.
- Nataša Kovačević, Anton Kokalj, "Analysis of molecular electronic structure of imidazole- and benzimidazole-based inhibitors: a simple recipe for qualitative estimation of chemical hardness", *Corros. sci.*, vol. 53, issue 3, pp. 909-921, 2011.
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#### REVIEW ARTICLES AND CHAPTERS IN BOOKS

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- Marjan Jereb, Dejan Vražič, Marko Zupan, "Iodine-catalyzed transformation of molecules containing oxygen functional groups", *Tetrahedron*, vol. 67, no. 7, pp. 1355-1387, 2011.
- Stojan Stavber, "Recent advances in the application of Selectfluor <sup>™</sup> F-TEDA-BF<sub>4</sub> as a versatile mediator or catalyst in organic synthesis", *Molecules (Basel)*, vol. 16, no. 8, pp. 6432-6464, 2011.

#### PUBLISHED CONFERENCE PAPERS

#### **Regular** papers

- Leon Bedrač, Jernej Iskra, "Oksidacija joda v jodove (I) spojine z vodikovim peroksidom", In: *Slovenski kemijski dnevi 2011, Portorož,* 14-16 september 2011, Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2011, 7 pp.
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#### TEXTBOOKS AND LECTURE NOTES

- 1. Ester Heath, Tina Kosjek, Jernej Iskra, David Heath, Tomaž Skapin, Extraction techniques for the green chemist: učno gradivo pri predmetu "Green Chemistry", Ljubljana, Jožef Stefan International Postgraduate School, 2011.
- Ester Heath, Tina Kosjek, Jernej Iskra, David Heath, Tomaž Skapin, Extraction techniques for the green chemist: učno gradivo pri predmetu "Tools for the environmental quality control - organic pollutant in the environment", Ljubljana, Jožef Stefan International Postgraduate School, 2011.

#### PATENT APPLICATION

1. Rok Zupet, Anica Pečavar, Jernej Iskra, Miloš Ružič, Ivanka Kolenc, *A process for a preparation of marbofloxacin and intermediate thereof,* W02011061292 (A1), World Intellectual Property Organization, 26.5.2011.

Rok Prebil, B. Sc.
 Peter Rodič, B. Sc.
 Dejan Vražič, B. Sc.
 Technical officers
 Barbara Kapun, B. Sc.
 *14. Mojca Seručnik, B. Sc., left 01.08.11* Gregor Žerjav, B. Sc.

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8

## 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 energy, mainly complex multifunctional materials and structures. The materials of interest include ceramic piezoelectrics, ferroelectrics, relaxors, multiferroics and conductive oxides. The emphasis is on the creation of these properties by the synthesis and structure at the nano-, micro- and macro-levels. The group also works on the principles of basic technologies for ceramic pressure sensors, ceramic MEMS and flexible electronics.

Within the research on environment-friendly, lead-free, piezoelectric ceramics the focus has been on alkali niobates. We have studied the linear thermal expansion behavior of the  $K_{0.5}Na_{0.5}NbO_3$  ceramic between room temperature and 790 °C by contact dilatometry. The material was single phase with a 95.5 % relative density and with a uniform microstructure. Three distinct regions of thermal expansion could be discerned, corresponding to the three phases of  $K_{0.5}Na_{0.5}NbO_3$ , i.e., monoclinic (assuming a single perovskite unit cell), tetragonal and cubic, separated by discontinuities, as is typical for the first-order phase transitions. The linear coefficient of thermal expansion between 30 °C and 195 °C is 2.96  $\cdot 10^6 \text{ K}^1$ , between 208 °C and 364 °C 4.35  $\cdot 10^6 \text{ K}^1$ , and between 434 °C and 790 °C 7.52  $\cdot 10^6 \text{ K}^1$ . These results can contribute to a better understanding and design of lead-free piezoelectric thick- and thin-film structures and devices. We have continued our research on the sintering of NaNbO, ceramics. The optimal

sintering conditions, which resulted in fine-grained ceramics with a high relative density, were determined. We investigated the equilibrium vapour pressures of sodium over selected compositions in different two-phase regions in the Na<sub>2</sub>O(Na<sub>2</sub>CO<sub>3</sub>)-Nb<sub>2</sub>O<sub>5</sub> system in collaboration with the Department of Environmental Sciences, JSI, and Eötvös Loránd University, Budapest, Hungary. The use of Knudsen effusion mass spectrometry (KEMS) between 1100 and 1470 K allowed us to determine the standard thermodynamic functions of the solid compounds Na<sub>3</sub>NbO<sub>4</sub>, NaNbO<sub>3</sub>, Na<sub>2</sub>Nb<sub>4</sub>O<sub>11</sub>, NaNb<sub>3</sub>O<sub>8</sub> and NaNb<sub>13</sub>O<sub>33</sub> (Figure 1). The high-temperature stability of sodium niobate under typical sintering conditions (e.g., 1350 °C, air atmosphere) was modelled and the results, which are in agreement with the experimental observations, are the basis for a further optimisation of the processing of alkali-niobate-based ceramics.

Within the activities on **lead-based piezoceramics**, the synthesis and characterization of composites composed of donor-doped lead zirconate titanate (PZT) and yttrium-stabilized tetragonal zirconia should be mentioned. Within the EU 7FP project HIPERact, in collaboration with Technische Universität Darmstadt and the Swiss Federal Institute of Technology, we found that the addition of zirconia influenced the phase composition, microstructure, dielectric, ferroelectric and piezoelectric properties of the composites. The

measurements of polarization and strain versus the electric field indicated that the zirconia particles in the PZT matrix act as pinning centers for ferroelectric domain switching. In addition, a reduced frequency dispersion and reduced non-linearity of the piezoelectric  $d_{33}$  coefficient in the composites also suggest a suppressed, non-180°, domain-wall contribution in these samples.

We further studied the ferroelectric and piezoelectric properties of **BiFeO**<sub>3</sub>. Since BiFeO<sub>3</sub> is receiving increased interest as a high-temperature piezoelectric, we studied in detail the electromechanical response of the ferrite under AC electric fields. A large bipolar strain of up to 0.36% was measured in BiFeO<sub>3</sub> ceramics at 140 kV/cm and 0.1 Hz. Such a value is comparable to the strain obtained in highly efficient, lead-based perovskites, such as Pb(Zr,Ti) O<sub>3</sub> (PZT) and Pb(Mg,Nb)O<sub>3</sub>-PbTiO<sub>3</sub> (PMN-PT). The strain showed a strong frequency dependence, i.e., increasingly larger strains were obtained at lower field frequencies (<10 Hz), which was attributed to the non-180° domain-wall switching. In addition, the rearrangement of defects at low-frequency fields



Prof. Marija Kosec

Head



Figure 1: Activities of Na<sub>2</sub>O at 1000 K, as calculated from the measured equilibrium vapour pressures over selected compositions in different solid two-phase regions of the Na<sub>2</sub>O-Nb<sub>2</sub>O<sub>5</sub> phase diagram. 3/1: Na<sub>3</sub>NbO<sub>4</sub> 1/1: NaNbO<sub>4</sub> 2/4: Na<sub>2</sub>Nb<sub>4</sub>O<sub>1</sub>p 1/3: NaNb<sub>3</sub>O<sub>8</sub> 1/13: NaNb<sub>13</sub>O<sub>33</sub>

The use of Knudsen effusion mass spectrometry (KEMS) between 1100 and 1470 K allowed us to investigate the equilibrium vapour pressures of sodium over selected compositions in different two-phase regions in the Na<sub>2</sub>O(Na<sub>2</sub>CO<sub>3</sub>)-Nb<sub>2</sub>O<sub>5</sub> system and to determine the standard thermodynamic functions of the solid compounds in this system. The results are the basis for further optimisation of the processing of alkali-niobate-based ceramics.



Figure 2: Strain-electric-field hysteresis loops of BiFeO<sub>3</sub> measured at different frequencies and electric field amplitudes.

effectively released these domain walls from the pinning centers, resulting in an enhanced response (Figure 2).

We continued our research work on the mechanisms of mechanochemical reactions, focusing on a comparison of the mechanochemical synthesis of NaNbO<sub>3</sub> and KNbO<sub>3</sub> from the respective alkaline carbonates and Nb<sub>2</sub>O<sub>5</sub>. While the mechanochemical formation of NaNbO<sub>3</sub> is realized at a relatively low ball-impact energy, the synthesis of KNbO<sub>3</sub> is rather complex. A quantitative phase analysis of the powders using the Rietveld refinement method revealed the formation of KNbO<sub>3</sub> in the initial stage of milling, which upon further milling decomposed to a K<sub>2</sub>Nb<sub>4</sub>O<sub>11</sub>-like phase. The fraction of this phase in the "quasi" equilibrium, i.e., when the steady-state milling conditions were reached, depended only slightly on the ball-impact energy. Similarly, high-energy milling of pre-formed KNbO<sub>3</sub> resulted in the decomposition of the perovskite to a potassium-deficient phase, which could be understood in terms of the instability of KNbO<sub>3</sub> under high-energy ball-impacts.

Furthermore, the 0.57Pb(Sc<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub>-0.43PbTiO<sub>3</sub> (PSN-PT) ceramic was prepared. This ceramic, with its Curie temperature of 270 °C, is suitable for applications below ~ 200 °C. The ceramic powders were prepared by

mechanochemical activation and sintered to 97 % relative density at 1000 °C, which is 200–300 °C lower than the temperatures reported in the open literature. We showed that the dielectric, ferroelectric and piezoelectric properties of such ceramics are comparable to the properties of niobium-doped PSN-PT ceramics and Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)  $O_3$ -PbTiO<sub>3</sub> ceramics (Figure 3).

KTaO<sub>3</sub> is an archetypal, incipient ferroelectric, in which long-range ferroelectric order does not establish at low temperatures owing to quantum fluctuations. Due to the extremely demanding processing the reports about ceramics and thin films have only recently started to emerge. We have prepared polycrystalline **KTaO<sub>3</sub>** thin films on (0001) sapphire by **Chemical Solution Deposition**. In collaboration with the Institute of Physics of the Academy of Sciences of the Czech Republic from Prague, we analyzed the films with microwave and terahertz spectroscopies. The soft-mode behavior is clearly observed in the THz spectra with a frequency minimum at 60 K. At the same temperature a permittivity maximum in the microwave range appears. The THz spectra strongly resemble those of strained epitaxial SrTiO<sub>3</sub>/DyScO<sub>3</sub> films. The described properties give strong evidence for the ferroelectric phase transition near 60 K, which has been observed in polycrystalline KTaO<sub>4</sub> films for the first time.

 $\label{eq:Research} Research of lead-free, potassium sodium niobate (K_{0.5}Na_{0.5})NbO_3 thin films on Pt(111)/TiO_2/SiO_2/Si substrates from the acetate-alkoxide-based precursor sols with the stoichiometric composition and with 5 mol % or 10  



Figure 3: a) Microstructure of 0.57PSN-0.43PT ceramic sintered at 1000 °C, with 97 % relative density. b) The measured (black dots), calculated (line) and difference curves (line bottom) of the X-ray diffraction pattern of the 0.57PSN-0.43PT ceramic. The tick marks represent the reflections of the tetragonal and monoclinic phases. In brackets, the families of diffraction peaks of the perovskite phase are shown. c) Dielectric constant of 0.57PSN-0.43PT ceramic vs. temperature. d) Ferroelectric hysteresis loop of the 0.57PSN-0.43PT ceramic.

% excess of sodium or potassium acetate continued. The microstructure of about 250-nm-thick films, rapid thermally annealed at 750 °C prepared from the stoichiometric and 5 mol % excess solutions consists of equiaxed grains of about 50 nm across, while the grain size in the about 220-nm-thick films prepared from the 10 mol % excess solutions is about 200 nm. The energy-dispersive X-ray spectroscopy (EDXS) in a field-emission scanning electron microscope revealed that the alkali excess in precursor solutions contributed to a higher level of chemical homogeneity of the films on the micron scale. The films prepared from the 5 % potassium excess solution had the chemical composition closest to the nominal one among all the samples and they exhibited room-temperature values of the dielectric permittivity, dielectric losses, remnant polarization and coercive field measured at 1 kHz 610, 0.015, 8  $\mu$ C/cm<sup>2</sup> and 80 kV/cm, respectively (Figure 4).

The aim of **transparent electronics** is the realization of fully transparent devices, which could be used in applications such as flat-panel displays. This requires the deposition of semiconducting or dielectric thin films with suitable properties onto substrates requiring low-temperature processing, such as glass or polymer foils. High-K dielectric  $Ta_2O_5$ ,  $Al_2O_3$ , and  $SiO_2$ -based thin films on glass were processed by Chemical Solution Deposition and heated at 450 °C. The about 100-nm-thick XRD amorphous films were characterized by a low roughness, with RMS < 0.3 nm. The dielectric permittivity values of the binary or ternary amorphous compositions are lower than those of the  $Ta_2O_5$  films. In contrast, compared to the  $Ta_2O_5$  films, an improvement in the

transparency in the visible range was observed for binary or ternary compositions. The work was performed in the frame of the EU 7FP project ORAMA.

PZT thick films on flat substrates are applicable in high-frequency ultrasound transducers for medical diagnostics. To improve the sensitivity of the devices, the PZT films should be deposited on curved ceramic substrates. Electrophoretic deposition (EPD) was used to prepare PZT thick films on both flat and curved substrates. We investigated the influence of the ethanolbased dispersion properties and the deposition conditions on the uniformity of the deposits. We systematically studied the microstructure of the thick films as a function of the deposition and sintering conditions (temperature, time, packing powder). The research in collaboration with François Rabelais University from Tours, France, revealed that EPD was a suitable method for the processing of thick-film structures on curved substrates.

We prepared PZT thick films on silicon and alumina substrates by inkjet printing. PZT particles were stabilized in water at different pH values using polyacrylic acid (PAA). During milling, the PZT particle size decreased and the amount of PAA adsorbed on the particles increased at pH >7. The adsorption was studied by infrared spectroscopy in collaboration with the "Ilie Murgulescu" Institute of Physical Chemistry from Bucharest, Romania. Under optimal processing conditions we prepared aqueous PZT dispersions with a median particle size  $d_{v_{50}}$  = 170 nm and a zeta-potential of -50 mV. The optimal addition of the selected surfactant and the binder resulted in a dispersion with a viscosity of 10 mPas (at 100  $s^{-1}$ ) and a surface tension of 30 mN/m. These dispersions were used for patterning the structures with a piezoelectric ink-jet printer.

Within the EU 7FP project MICROFLEX a water-based PZT ink for printing on flexible substrates was developed. After ink-jet printing and drying, the porous PZT film was additionally impregnated by acrylate monomers, and UV-cured, which resulted in an enhanced stability of the PZT film. The process is suitable for the realisation of piezoelectric sensors and actuators on flexible substrates.

We have prepared K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> (KNN) thick films by screen-printing. KNN was synthetized by solid-state reaction. The sintering temperature of the thick films was reduced to 1000°C, which was achieved by the addition of 1. The error bars indicate  $\pm 1\sigma$  standard deviation. For guidance, the alkali germanates or alkali carbonates, which serve as liquid-phase sintering aids at high temperatures. Thick films have a crystallographic orientation in the (100) direction and less in the (10-1) direction.



Figure 4: Plots of the K/Na and (K+Na)/Nb atomic ratios, calculated from the experimental data for each investigated  $K_{0.5}Na_{0.5}NbO_3$  (KNN) thin film. The full line shows the stoichiometric (K+Na)/Nb atomic ratio = 1. The dotted line shows the K/Na atomic ratio in the sols, reflecting the amount and the chemical composition of the alkali excess in the sols. Note that the K/Na atomic ratio of the KNN perovskite phase is equal to data for the film prepared from the stoichiometric sol (St-I, St-II) are highlighted. On the top, the microstructures of the films prepared from 5 and 10 mol % potassium excess sols are added.

We studied the processing of oriented 0.65Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-0.35PbTiO<sub>3</sub> (PMN-PT) thick films by screenprinting. The cubic PMN-PT templates, prepared by a solid-state synthesis, were added into the thick-film paste. The processing of the templates and the screen-printing are both low-cost procedures and could be potentially used in industry.

Investigations of LTCC (low temperature co-fired ceramics) materials used for the realisation of multilayer circuits and 3D structures with buried cavities (MEMS - Micro Electro Mechanical Systems) continued. One of the most widely used LTCC tapes, DuPont 951, was thoroughly investigated. The influence of the phase composition on the characteristics of these LTCC tapes heated under different conditions was studied. The propagation of cracks through the as-sintered LTCC tapes was investigated. In the tapes heated at lower temperatures the cracks propagate through the glassy phase and continue through the pores, while in the tapes heated at higher temperatures, which have a significantly lower fraction of porosity, the cracks still propagate through the glassy phase, but they are deflected by embedded alumina grains. Upon heating at even higher temperatures, the glassy phase,

Measurements of the electromechanical response of BiFeO<sub>3</sub>, which is receiving an increasing interest as a material for hightemperature piezoelectric applications, revealed a large electric-field-induced strain (0.36%), comparable to that achieved in lead-based perovskites. We attribute this strain to the non-180° domain-wall switching and rearrangement of defects under the electric field, which further increases the mobility of such domain walls.

surrounding the alumina grains, partially crystallises into the anorthite phase. In this case, the cracks propagate through the glassy and anorthite phases.

Two new LTCC materials, i.e., Heraeus CT 702 and Ferro L8, were evaluated. In both cases the glass phase partially crystallised upon heating, resulting in better mechanical properties of the LTCC structures. Scanning electron



*Figure 5: The ceramic pressure sensor for the low-pressure range 0-30 mbar, with a sensitivity of 0.05 mbar.* 

microscopy revealed a higher concentration of glassy phase in the Heraeus CT702 as compared to the Ferro material, which explains its lower flexural strength. The electrical characteristics of different **thick-film resistors** processed on the LTCC substrates (Heraeus CT702, Ferro L8 and DuPont 951) were investigated in collaboration with the

partner HIPOT-RR. The thick-film resistors were heated after deposition on either "green" or pre-fired LTCC tapes. Sheet resistivity, noise, temperature coefficients of resistivity (TCR) and gauge factors were measured. The best results were obtained on the Du Pont LTCC 951, with the noise below 0.1 mV/V, TCRs below 100x10<sup>6</sup>/K and gauge factors around 10.

Within the co-operation with the "Tele and Radio Research Institute" and the "Warsaw University of Technology" the realisation of narrow, thick-film, conductor lines on LTCC substrates by ink-jet printing technology was studied. The aim was the miniaturisation of the LTCC structures. Silver-based conductor lines heated at 850°C with a width of 70-100 mm, a thickness of 4 mm and a sheet resistivity of 4.5 m $\Omega$ / $\Box$ , were realised on the pre-fired LTCC substrates.

The technology for producing thin membranes and relatively large buried cavities in the 3D LTCC structures was developed in cooperation with the research partner HIPOT-RR. The level of the developed technology enables the industrial and the research partners HYB d.o.o. and IN.Medica

d.o.o. to design and to develop prototypes of ceramic pressure sensors for wide ranges of pressures from 0-100(30) mbar to 0-34(100) bar. The **ceramic pressure sensor** for the low pressure range 0-30 mbar with the sensitivity of 0.05 mbar was an important achievement of the partners (Figure 5).

In cooperation with colleagues from Vienna Technical University within the scope of the project EUREKA: New generation of 3D Integrated Passive Components and Microsystems in LTCC Technology – IPCTECH, the structural characteristics of ferromagnetic LTCC tapes, heated at different temperatures, were investigated by X-ray powder diffraction analysis, scanning electron microscopy and EDXS analysis. The nominal permeability of the tapes based

By employing various broad-band dielectric spectroscopy methods we have obtained strong evidence for the existence of the lowtemperature ferroelectric state of KTaO<sub>3</sub> thin films on (0001) sapphire substrates. The induced ferroelectricity in polycrystalline KTaO<sub>3</sub> films prepared by Chemical Solution Deposition has been confirmed for the first time.

on  $(Ni_{0.35}Zn_{0.65})Fe_2O_4$  was around 450.

In cooperation with the factory ETI d.d. Izlake, we studied materials based on steatite, which are used for the manufacture of various electrical components. The aim of the research was to improve the mechanical and thermal properties of the steatite. Improved properties were achieved by replacing selected raw materials, optimising the amount of the additives, and optimised the milling and heating. The modified procedure for the preparation of the steatite has been successfully used for the manufacture of complex electrical products, such as housings for fuses.

#### Some outstanding publications in the last year

- Volodymyr Skoromets, Sebastjan Glinšek, Viktor Bovtun, Martin Kempa, Jan Petzelt, Stanislav Kamba, Barbara Malič, Marija Kosec, Petr Kužel, Ferroelectric phase transition in polycrystalline KTaO<sub>3</sub> thin film revealed by terahertz spectroscopy. Appl. phys. lett., 99 [5], (2011), 052908-1-052908-3.
- Jenny Tellier, Barbara Malič, Danjela Kuščer, Gregor Trefalt, Marija Kosec, Ink-jet printing of In<sub>2</sub>O<sub>3</sub>/ZnO twodimensional structures from solution. J. Am. Ceram. Soc., 94 [9], 2011, 2834-2840.
- Gregor Trefalt, Barbara Malič, Danjela Kuščer, Janez Holc, Marija Kosec. Synthesis of Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub> by selfassembled colloidal aggregates. J. Am. Ceram. Soc., 2011, 94 [9], 2846-2856.

#### Awards and appointments

- 1. Alja Kupec, best student poster, COST MP0904 SIMUFER, Hasselt, Belgium, March 23, 2011
- 2. Gregor Trefalt, acknowledgment for the presentation: Innovative Approach to Synthesis of Pb(Mg1/3Nb2/3)O3 Based Materials Using Colloidal Interactions, the 3rd Jožef Stefan International Postgraduate School Students Conference, IPS, Ljubljana, Slovenia, May 25, 2011
- 3. Marija Kosec, MIDEM acknowledgement, the ceremony at the 25th Academy of the Society for Microelectronics, Electronic Components and Materials, Ljubljana, Slovenia, May 26, 2011
- 4. Jurij Koruza, award for the presentation in the section of young researchers (anorganic materials field): Microstructure Development upon Two-Stage Sintering of Nano-Sodium Niobate, 19. konferenca o materialih in tehnologijah, Portorož, Slovenia, November 23, 2011

#### Annual Report 2011

#### Organization of conferences, congress and meetings

- 1. Joint seminar NETZSCH, Kemomed d.o.o., Jožef Stefan Institute and Centre of Excellence NAMASTE: Modern Thermoanalytical Techniques and their Application, Ljubljana, Slovenia, June 7, 2011
- SEMTO Conference 2011: Napredni materiali s tehnologijami prihodnosti, Ljubljana, Slovenia, September 7-8, 2011
- 3. E-MRS Fall Meeting, Symposium: Solution-derived electronic-oxide films, nanostructures and pattering, from materials to devices, Warsaw, Poland, September 19-22, 2011

## INTERNATIONAL PROJECTS

- 1. Oxide Materials Towards a Matured Post-silicon Electronics Era
  - ORAMA 7. FP, NMP3-LA-2010-246334

EC; Dr. Bernd Szyszka, Head of Department Large Area Coating, Fraunhofer Institute for Surface Engineering and Thin Films (IST), Braunschweig, Germany; Fraunhofer-Gesellschaft zur Foerderung der Angewandten Forschung E.V., Muenchen, Germany Prof. Marija Kosec, Prof. Barbara Malič

- 2. Micro Fabrication Production Technology for MEMS on New Emerging Smart Textiles/ Flexibles
  - MICROFLEX

7. FP, NMP2-LA-2008-211335

EC; Dr. Steve Beeby, University of Southampton, School of Electronics and Computer Science, Hampshire, Southampton, Great Britain

- Prof. Marija Kosec, Dr. Janez Holc, Prof. Tomaž Kosmač 3. Novel Technology for High-PERformance Piezoelectric Actuators
  - HIPER-Act
  - 7. FP
  - CP-IP 212394, FP7-NMP-2007-LARGE-1
  - EC; Anders Brezen, Noliac A/S, Kvistgaard, Denmark
  - Prof. Marija Kosec, Asst. Prof. Andreja Benčan Golob
- SIMUFER: Single- and Multiphase Ferroics and Multiferroics with Restricted Geometries COST MP0904
  - EC; COST Office, Brussels, Belgium Prof. Barbara Malič, Dr. Tadej Rojac
- Integration and Control of Liquid Fuel Processor on Ceramic Micro-systems CERACON
  - ESA PECS, 4000103742/11/NL/KML

Bernard Zufferey, ESA-The European Space Agency, Paris, France; European Space Research and Technology Centre, Noordwijk, The Netherlands

- Asst. Prof. Marko Hrovat, Dr. Gregor Dolanc 6. New Generation of 3D Integrated Passive Components and Microsystems in LTCC Technology
  - IPCTECH
  - EUREKA Asst. Prof. Marko Hrovat
- Low Temperature Processing of Functional Oxide Thin Films
- Low Temperature Processing of Functional Oxide Thin Films BI-FI/11-12-001 Asst. Prof. Marina Tyunina, University of Oulu, Microelectronics and Materials Physics

Laboratories, Oulu, Finland prof. dr. Barbara Malič

 Lead-free Piezoelectric Ceramics based on Alkaline Niobates/Tantalates: Study of Synthesis, Structure and Phase Transition BI-FR/10-11-PROTEUS-003 Dr. Brahim Dkhil, Ecole Centrale Paris, Chatenay-Malabry, France

Dr. Brahim Dkhil, Ecole Centrale Paris, Chatenay-Malabry, France Prof. Barbara Malič

9. Studies on Structure-Properties Relationship of Novel Electronic Ceramics BI-CN/09-11-001 Prof. Hong Wang, Xi'an Jiaotong University, Xi'an, China Prof. Marija Kosec

- Investigation of Advanced Deposition Technologies for Interconnections in Organic and Flexible Electronics
  - BI-PL/10-11-013

Prof. Janusz Sitek, Tele and Radio Research Institute, Warsaw, Poland Asst. Prof. Danjela Kuščer Hrovatin

- Study of Novel Synthesis Routes of Environment-friendly Complex Oxides BI-RO/10-11-005
   Prof. Maria Magdalena Zaharescu, Ilie Murgulescu Institute of Physical Chemistry,
  - Prof. Maria Magdalena Zanarescu, nie Murgulescu Institute of Physical Chemisury, Bucharest, Romania Prof. Barbara Malič
- Studies of the Processing Influence on Functional Properties of Ferroelectric Materials for Microwave Applications BI-US/11-12-002

Dr. Angus Kingon, Brown University, Providence, RI, USA Prof. Marija Kosec

## R & D GRANTS AND CONTRACTS

- Functional properties of thin films based on environment friendly complex perovskite materials: dependence on microstructure and chemical homogeneity Prof. Barbara Malič
- Textured Ceramic Films for Sensors and Actuators Prof. Marija Kosec
- Oxide-based components for transparent electronics Prof. Barbara Malič
- 4. Energy-saving ceramic pressure sensors with digital output Asst. Prof. Marko Hrovat
- 5. Processing of ceramic microelectromechanical systems (MEMS) by novel technologies Dr. Janez Holc
- 6. Ceramic materials for 3D structures and study of functional properties-cofinancing
- Dr. Janez Holc 7. Materials and technologies for chemical microsystems
- Dr. Janez Holc
- 8.  $Pb(Sc_{0,5}Nb_{0,5})O_3-PbTiO_3$  thick films for sensor and actuator applications Dr. Hana Uršić Nemevšek

## RESEARCH PROGRAM

1. Electronic Ceramics, Nano-, 2D and 3D Structures Prof. Marija Kosec

## MENTORING

#### Ph. D. Thesis

1. Roman Pačnik, Hydraulic load cells for measurement of small loads (mentor Franc Novak; co-mentor Marija Kosec).

#### Bologna M. Sc. Thesis

1. Helena Razpotnik, Researches of porcelain scrap application in alumina porcelain C-120 (mentor Marija Kosec; co-mentors Janez Holc, Ivan Lavrač).

## VISITORS FROM ABROAD

- Prof. Angus Kingon, Brown University, Rhode Island, USA, January 17 21, 2011
   Dr. Valentina Cauda, Center for Space Human Robotics-IIT@PoliTO, Torino, Italy,
- January 31 February 4, 2011
- Steve Muckett, Mozaik Technology Ventures Ltd, London, UK, February 22, 2011
   Prof. Klaus Reichmann, Institute of Chemistry and Technology of Materials, Graz
- University of Technology, Graz, Austria, April 15, 2011 5. Prof. Angelika Reichmann. Institute of Electron Microscopy
- Prof. Angelika Reichmann, Institute of Electron Microscopy and Fine Structure Research, Graz University of Technology, Graz, Austria, April 15, 2011
   Bensemma Nouar, Neutron Scattering Department, Nuclear Research Center of F
- Bensemma Nouar, Neutron Scattering Department, Nuclear Research Center of Berine, Djelfa, Algeria, April 21 – July 21, 2011
- 7. Prof. Vlasta Sedlakova, Prof. Jozef Sikula, Dr. Petr Sedlak, Dr. Jiri Majzner, Physics

Department, Faculty of Electrical Engineering and Communication, Brno University of Technology, Brno, Czech Republic, May 9 - 11, 2011

- Prof. Marina Tjunina, University of Oulu, Microelectronics and Materials Physics Laboratories, Oulu, Finland, May 16 – 22, 2011
- Prof. Franck Levassort, Francois-Rabelais University of Tours, Tours, France, May 18 20, 2011
- 10. Prof. Mamoru Senna, Keio University, Keio, Japonska, July 6 October 10, 2011
- Prof. Janusz Sitek, Tele and Radio Research Institute, Warsaw, Poland, September 27 30, 2011
- 12. Konrad Futera, Tele and Radio Research Institute, Warsaw, Poland, September 27 30, 2011
- Prof. Hisao Suzuki, Shizuoka University, Shizuoka, Japan, September 24 October 1, 2011
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- Dr. Oana Catalina Mocioiu, Ilie Murgulescu Institute of Physical Chemistry, Bucharest, Romania, October 10 – 22, 2011
- 17. Dr. Marco Deluca, Institut für Struktur- und Funktionskeramik, Montanuniversitaet Leoben, Loeben, Austria, October 21, 2011
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- 18. Evgeniya Khomyakova, B. Sc.
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- C. Hubault, C. Davoisne, Löic Dupont, A. Perrin, A. Boulle, Janez Holc, Marija Kosec, Michael Gordon Karkut, Nathalie Lemée, "Inhibition of polydomain formation in PbTiO<sub>3</sub>/PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub> superlattices by intercalation of ultra-thin SrTiO<sub>3</sub> layers", *Appl. phys. lett.*, vol. 99, no. 5, pp. 052905-1-052905-3, 2011.
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### PUBLISHED CONFERENCE PAPERS

#### **Invited Papers**

- Darko Belavič, Marko Hrovat, Gregor Dolanc, Janez Holc, Marina Santo-Zarnik, Primož Fajdiga, Kostja Makarovič, Stanko Hočevar, Jurka Batista, Iztok Stegel, "A chemical microreactor as an example of an LTCC-based ceramic microsystem", In: *Proceedings*, Electronic Devices and Systems, [EDS'11] IMAPS CS International Conference, June 22-23, 2011, Brno, Czech Republic, Ondrej Hegr, ed., Brno, Vysoké učeni technické, 2011, pp. XIII-XVIII.
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#### Regular papers

- Andre-Pierre Abellard, Danjela Kuščer, Janez Holc, Franck Levassort, Oleksandr Noshchenko, Marc Lethiecq, Marija Kosec, "Fabrication aod modeling of piezoelectric transducers for High-Frequency medical imaging", In: *Proceedings*, 47th International Conference on Microelectronics, Devices and Materials and the Workshop on Organic Semiconductors, Technologies and Devices, September 28 - September 30, 2011, Ajdovščina, Slovenia, Gvido Bratina, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2011, pp. 33-37.
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- 3. Darko Belavič, Marko Hrovat, Gregor Dolanc, Stanko Hočevar, Iztok Stegel, Marina Santo-Zarnik, Janez Holc, Kostja Makarovič, Jurka Batista, Primož Fajdiga, Marija Kosec, "Design and fabrication of a complex LTCC-based reactor for the production of hydrogen for portable PEM fuel cells", In: *Proceedings*, 2011 IMAPS/ACerS, 7th International Conference and Exhibition on Ceramic Interconnect and Ceramic Microsystems Technologies (CICMT), April 5-7, 2011, San Diego, California, USA, Washington, International Microelectronics and Packaging Society, 2011, pp. 23-28.
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- 5. Darko Belavič, Marina Santo-Zarnik, Marjan Hodnik, Sandi Kocjan, Marko Hrovat, Kostja Makarovič, "Temperature behavior of LTCCbased pressure sensors", In: *Proceedings*, 47th International Conference on Microelectronics, Devices and Materials and the Workshop on Organic Semiconductors, Technologies and Devices, September 28 - September 30, 2011, Ajdovščina, Slovenia, Gvido Bratina, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for

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#### THESES

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1. Janez Holc, Kostja Makarovič, Darko Belavič, Marko Hrovat, Marija Kosec, Boris Jordan, *The method of fabrication of buried cavities in multilayer ceramic structures*, P-201100202, Urad RS za intelektualno lastnino, 3.6.2011.

## **ENGINEERING CERAMICS** DEPARTMENT

The Engineering Ceramics Department is the leading group in the field of structural ceramics and ceramic technologies in Slovenia. The research programme comprises the phenomena relevant to the materials synthesis and component fabrication as well as the mechanisms leading to a degradation of engineering 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 environment-friendly ceramic technologies.

In 2011 we continued our research on the degradation of aluminium-nitride (AlN) powder in water in terms of the hydrolysis process. This time we carefully followed the evolution of aluminum hydroxides in diluted aqueous AlN-powder suspensions in the temperature range of 22–90°C in order to set up a general mechanistic model over a broad temperature range, uniting previously observed hydrolysis reactions at room temperature and at elevated temperatures into a single scheme. We showed that dispersing the AlN powder in the water results in the temperature-Head dependent formation of various aluminum hydroxides in the following sequence: amorphous aluminum hydroxide Prof. Tomaž Kosmač gel, aluminum monohydroxide (boehmite) and aluminum trihydroxides (bayerite, nordstrandite, and gibbsite). Based on these findings, along with the understanding of the hydrolysis reaction kinetics (which we studied previously), we exploited the hydrolysis for the preparation of the colloidal carrier powder with a high specific surface for the deposition of nanoparticles and/or thin films of a foreign material.

The colloidal carrier powder, consisting of micron-sized bundles of lamellar boehmite particles, can be subsequently transformed into one of the transitional aluminum oxides ( $\gamma$ -,  $\delta$ - or  $\theta$ -Al<sub>2</sub>O<sub>2</sub>) without a substantial change in the morphology before or after the deposition of the nanoparticles. The supporting colloidal powder is designed for the improved effectiveness and

properties of the films and/or particles exhibiting specific or improved properties due to its high specific surface area and porosity. This was shown feasible in the case of TiO<sub>2</sub>, where the nanostructured  $\gamma$ -Al<sub>2</sub>O<sub>2</sub>/TiO<sub>2</sub>-composite powder exhibited up to 3-times-higher photo-activity in the near-UV region compared to commercially available TiO<sub>2</sub> nanoparticles. The procedure was issued with a Slovenian patent application.

In the frame of the research on thermoplastic ceramic suspensions we studied the removal of a binder from the low-pressure injection-molded part. Our 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 the paraffin ceramic suspensions in the range of 40-60 vol% of the powder content, taking into account the particle-size distribution, the type of material and the distance between the particles in the suspension.

In the field of electrically conductive ceramic composites we continued, in 2011, with the research on the preparation and the properties of composites based on silicon nitride  $(Si_{a}N_{a})$  with the dispersed titanium nitride (TiN) and zirconium nitride (ZrN) particles. The Si<sub>x</sub>N<sub>4</sub>/TiN and Si<sub>x</sub>N<sub>4</sub>/ZrN composites were prepared by forming the conductive TiN or ZrN nano-particles on the  $Si_2N_4$ -powder surface with the gel-precipitation of hydroxides and

the subsequent thermal treatment. After calcination at 600°C in air metallic hydroxides were transformed to crystalline oxides (TiO<sub>2</sub> and ZrO<sub>2</sub>). At 900°C in an NH, gas flow TiO, reacted with NH, to form TiN and at 1600°C the ZrO, particles reacted with Si<sub>2</sub>N<sub>4</sub> to form ZrN. To fabricate electrically conductive Si<sub>2</sub>N<sub>4</sub>/TiN composites, the Si<sub>2</sub>N<sub>4</sub> powders coated with various amounts of nano-sized nitride particles were sintered together with yttria and alumina

The research on binder removal in a highly porous carbon powder has indicated a new process for removing the binder, which was also patented.

additives at 1850°C for 2 h in nitrogen atmosphere. The results of measurements of the electrical conductivity and flexural strength demonstrated that the sintered composites containing various TiN or ZrN contents make these ceramics suitable for the production of heating elements at a lower vol. % of the conductive phase. We also investigated the possibility of preparing the Si,N/ZrN composites by directly sintering the Si,N/-powder-coated ZrO, nanoparticles with the Y<sub>2</sub>O, and Al<sub>2</sub>O, additives. In this case we expected the reaction between ZrO<sub>2</sub> and Si<sub>2</sub>N<sub>4</sub> to expire during the heating of the sample to a sintering temperature. However, in the composite with 20 vol. % of ZrO<sub>2</sub> in the initial formation of a mixture of grains the reaction between ZrO<sub>2</sub> and Si<sub>2</sub>N<sub>4</sub> did not expire until the

In 2011 we patented the process of preparing a colloidal carrier powder with a high specific surface area.



Figure 1: TEM micrographs of (a) AlOOH lamellas formed on the surface of the hydrolyzing AlN particle, (b) bundles of aggregated AlOOH lamellas formed after the hydrolysis of the AlN powder, (c) a nanostructured  $\gamma$ Al2O3/TiO2-composite particle and (d) an individual  $\gamma$ Al2O3/TiO2-composite lamella.

end. Notwithstanding the difference in the density from the core to the outer surface of the composite, the sample has a high flexural strength and electrical conductivity on the surface, while the inner part of the composite is an insulator. Based on the results, we concluded that such a promising process for manufacturing heating elements should be a one-step patented process for manufacturing composite ceramic heaters.

The research and development of dental ceramics based on tetragonal zirconia (Y-TZP)  $ZrO_2$  was conducted in two main directions. The investigation of the phase instability of the conventionally sintered dental 3Y-TZP ceramics in simulated clinical conditions was continued. The sintered samples in the shape of discs were exposed to accelerated ageing in an artificial saliva solution at 134°C. The zirconia-phase transformation from tetragonal to monoclinic was monitored with regard to the ageing time. The influence of the material and the processing variables on the transformation rate was investigated and the effect of mechanical surface treatment and accelerated ageing on the survival rate during the cyclic mechanical loading (fatigue testing) was evaluated. In order to estimate the expected lifetime of dental restorations from Y-TZP ceramics, the in-vivo experiments of ageing of materials were designed in cooperation with the dentists from the Medical

Faculty: two pairs of sintered ceramic discs were mounted into the lingual part of a removable denture and the relative amount of transformed monoclinic zirconia is determined every six months and compared with the results of the in-vitro tests of accelerated ageing in the artificial saliva. In 2010, six patients were included in this study and the results, after 24 months, indicate that the kinetics of ageing of dental Y-TZP ceramics in the mouth cavity is substantially different from the kinetics of accelerated ageing under isothermal conditions.

Part of the research on the dental ceramics was aimed at studying the influence of the nanostructured aluminate coating on the bonding strength of the dental cements of the dental ceramics based on Y-TZP and Ce-TZP/

A new, one-step manufacturing process for manufacturing composite ceramic heaters was developed and patented.  $Al_2O_3$ . The coatings were prepared by 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, they have a very high specific surface area and are strongly bonded to the ceramic surface. The results of the adhesion measurements showed that

aluminate coating improves the bonding strength by more than 100%, and that the strength is retained even after the termocycling of the samples, which is not the case with the samples without the coating, as they spontaneously debonded during the termoclycling test.

The research on the porous yttria-stabilized tetragonal zirconia (Y-TZP) ceramics for dental application was continued aiming at reducing the elastic modulus, while preserving a useful strength for the application in dental



Figure 2: Results of Monte-Carlo simulations of the agglomeration between the "core" and the "shell" Y-TZP particles influenced by the KCl concentration in the suspension.

medicine. The preparation of the so called "core-shell" composite is based on the aggregation of particles of various sizes of the same material in a suspension which results in a homogeneous distribution of the nano-sized particles attached to the surface of the submicron-sized particles. Due to a poor repeatability of the preparation of the "core-shell" nanocomposites, in the year 2011, we returned back to the basics, i.e., to the study of colloidal processing. Based on the previously obtained experimental data on the ZrO<sub>2</sub>–ZrO<sub>2</sub> system, a series of Monte-Carlo simulations of the agglomeration between the "core" and the "shell" Y-TZP particles, under various conditions, were performed. The simulations answered some of the important questions. At the moment we can say that the surface coverage of the micrometer particles with smaller nanometric particles depends on the solid loading of

the suspension, the pH, and the ionic strength of the suspension. It is an ongoing research on how to better control the agglomeration process that is at present quite coincidental.

In 2010 the investigations in the field of synthesis of bioactive calcium phosphate coatings on the zirconia Y-TZP substrates were continued. This Y-TZP ceramic is, due to its aesthetical and mechanical properties, frequently used in medicine as a material for dental implants. The fixation of an implant can be improved if its surface is covered with a bioactive calcium-phosphate coating that forms a strong bond with the bone tissue. The coatings were prepared by using a biomimetic method, in which the ceramic substrate is immersed in a solution with same physiological temperature and a composition similar to the human blood plasma. The crystallization of calcium phosphates from the aqueous solutions is a complex process, as the smallest change in the synthesis conditions
can influence the properties of the formed crystals, such as composition, crystal structure, morphology etc. For this reason the influence of various parameters (temperature, pH, solution composition, time of synthesis) on

the synthesis of coatings was researched. The obtained results enable us to control the synthesis of the coatings - by changing the conditions, the coatings with the desired properties can be synthesized.

The research on improving the wear resistance of the titanium alloys used for the preparation of bone implants was also continued. After nitriding at elevated temperatures (600-900 °C) in an ammonia atmosphere, a 100 to 300-nm-thick layer of titanium nitride was formed on the surface of the metallic titanium and its alloys. This has significantly increased the surface hardness and, consequently, improved the wear resistance of the material. The application of the titanium-nitride layers on the surface of metals increasing the hardness and thereby improving the wear resistance is known and often used, especially in the case of manufacturing 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 of the coating prepared by nitriding in ammonia is better than the TiN coating prepared with the PVD method. The wear rate of titanium and its alloys, to which we deposited a TiN layer with the PVD method after having been pitrided in the atmosphere of



Figure 3: FEG-SEM micrograph of a fracture surface of a titanium-alloy sample nitrided in an ammonia atmosphere at 900°C for 2 hours. A 150-nm-thin layer composed of titanium nitride was formed on the surface of the alloy.

layer with the PVD method after having been nitrided in the atmosphere of ammonia, was reduced by two thirds. The research in the frame of the project »Ageing of dental zirconia (Y-TZP) ceramics under simulated clinical conditions« was co-financed by the Interdent company from Celje, which intended to set up a production plant for manufacturing the pre-sintered ceramic blocks for the CAD-CAM milling of dental restorations. During the technological research two commercially available granulates of zirconia powder with the same chemical composition, but different average sizes of primary crystallites and different specific surface areas, were used. The processing variables were the pressure of the uniaxial dry pressing, the time and the temperature of pre-sintering influencing the strength and workability of semi-manufactured products and shrinkage, during sintering, to final density. The influence of these variables on the mechanical strength and the thermodynamic stability of the sintered ceramics under accelerated ageing conditions was investigated.

For the company called Dentas, d.o.o. from Maribor, manufacturing, in addition to milling machines and other equipment for dental laboratories, also the presintered blocks of zirconium oxide, we conducted some preliminary

research in the frame of a diploma work. The aim was to produce in-situ toughened mullite ceramics that would be suitable for a rapid firing of dental restorations. The mullite powder was sintered in the presence of a reactive transient liquid phase with the additives from the system  $Y_2O_3/La_2O_3$  - SiO<sub>2</sub>

# In 2011 we cooperated with many research institutions and industrial partners.

-  $Al_2O_3$ , which led to an anisotropic growth of the mullite grains in the form of intertwined sticks. The material has an improved resistance to rapid temperature changes; however, the mechanical strength is influenced by the presence of large pores generated during the reaction sintering.

The EU 7FP project called AppliCMA – "Development of wear resistant coatings based on complex metallic alloys for functional applications", in which the JSI is one of the partners, was finished in 2011. In the frame of this project we were in charge of the synthesis of the super-hard  $AlMgB_{14}$  compound, sintering of the powders and microscopic analysis of the products. The above mentioned compound was successfully synthesized and a solid sample used for a thin-film synthesis was prepared; however, they could not be used for the preparation of thin films, since the material did not withstand the conditions during the plasma-vapour deposition.

In cooperation with Hidria AET we developed a procedure for a rapid removal of the binder from the lowpressure injection-molded parts. This was achieved by using high-purity carbon black, which provides a capillary extraction in the first stage and does not interfere with the sintering process in the later stage. We also studied the strength distribution of alumina ceramic, in which case more than 5000 experimental measurements were taken into account. With this large number a fine statistical conclusion can be achieved. It was confirmed, that the Weibull distribution is indeed the best among the commonly used 2-parameter distributions.

#### Some outstanding publications in the past three years

 Kocjan Andraž, Dakskobler Aleš, Krnel Kristoffer, Kosmač Tomaž. The course of the hydrolysis and the reaction kinetics of AlN powder in diluted aqueous suspensions. J. Eur. Ceram. Soc.. [Print ed.], 2011, vol. 31, no. 5, pp. 815-823.

- Gorjan Lovro, Dakskobler Aleš, Kosmač Tomaž. Partial wick-debinding of low-pressure powder-injection-moulded ceramic parts. J. Eur. Ceram. Soc., 2011, vol. 30, no. 15, pp. 3013 – 3021.
- 3. Kocjan Andraž, Dakskobler Aleš, Kosmač Tomaž. Superhydrophobic nanostructured boehmite coatings prepared by AlN powder hydrolysis. International journal of applied ceramic technology, 2011, vol. 8, no. 4, pp. 848-853.
- 4. Gorjan Lovro, Dakskobler Aleš, Kosmač Tomaž. Strength evolution of injection-molded ceramic parts during wick-debinding. J. Am. Ceram. Soc., 2011, vol. 95, no. 1, pp. 188 193.
- 5. Dakskobler Aleš, Kocjan Andraž, Kosmač Tomaž. Porous alumina ceramics prepared by hydrolysis-assisted solidification. J. Am. Ceram. Soc., 2011, vol. 94, no. 5, pp. 1374-1379.
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- 7. Perko Sebastjan, Dakskobler Aleš, Kosmač Tomaž. High-performance porous nanostructured ceramics. J. Am. Ceram. Soc., 2010, vol. 93, issue 9, str. 2499-2502.
- 8. Jevnikar Peter, Krnel Kristoffer, Kocjan Andraž, Funduk Nenad, Kosmač Tomaž. The effect of nano-structured alumina coating on resin-bond strength to zirconia ceramics. Dent. Mater., 2010, vol. 26, no. 7, pp. 688-696.
- 9. Krnel Kristoffer, Kocjan Andraž, Kosmač Tomaž. A simple method for the preparation of nanostructured aluminate coatings. J. Am. Ceram. Soc., 2009, vol. 92, no. 10, pp. 2451-2454.
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## Patent granted

 Process for applying adhesion coatings to a substrate Tomaž Kosmač, Kristoffer Krnel, Andraž Kocjan, Peter Jevnikar EP2170244 (B1), European Patent Office, 30.3.2011.

## Awards and appointments

 Award for poster presentation on ECERS XII – 12th Conference of the European Ceramic Socience, 19-23 June 2011, Stockholm, Sweden; "Nano-structured aluminate coating improves self-adhesive resin cement bond to dental oxide ceramics", M. Golobič, A. Kocjan, T. Kosmač, P. Jevnikar

## Organization of conferences, congress and meetings

1. 5th Day of Young Researchers, Ljubljana, Slovenia, 17 February 2011

# INTERNATIONAL PROJECTS

- 1. Micro Fabrication Production Technology for MEMS on New Emerging Smart Textiles/Flexibles
  - MICROFLEX 7. FP, NMP2-LA-2008-211335
  - F. F. NMP 2-LA-2008-211555
    EC; Dr. Steve Beeby, University of Southampton, School of Electronics and Computer Science, Hampshire, Southampton, Great Britain
  - Science, Hampshire, Southampton, Great Britain Prof. Tomaž Kosmač, Prof. Marija Kosec, Dr. Janez Holc
- Development of Wear Resistant Coatings based on Complex Metallic Alloys for Functional Applications
  - appliCMA
  - 7. FP, 214407

EC; Andreas Merstallinger, Aerospace & Advanced Composites GmbH, Wiener Neustadt, Austria

Asst. Prof. Kristoffer Krnel, Asst. Prof. Miha Čekada, Prof. Janez Dolinšek, Asst. Prof. Srečo D. Škapin

# R & D GRANTS AND CONTRACTS

- 1. Patterns, Structural Self-assemly and Multiferroic States in Mixtures of Nanoparticles and Liquid Crystals
- Prof. Samo Kralj, Dr. Aleš Dakskobler 2. Research of dental ceramics
- Prof. Tomaž Kosmač

- Ageing of dental zirconia (Y-TZP) ceramics under simulated clinical conditions Prof. Tomaž Kosmač
- 4. Ceramic materials for 3D structures and study of functional properties-cofinancing Dr. Janez Holc, Prof. Tomaž Kosmač
- Phase-boundary investigations between bio-mimetically prepared calcium phosphate and Al2O3 or ZrO2 ceramics Dr. Irena Pribošič

# RESEARCH PROGRAM

1. Enigneering and bio-ceramics Prof. Tomaž Kosmač

# NEW CONTRACT

 Microstructure characterization and corrosion resistance of sintered dental ceramics Dentas Midhat Selimović S.p. Prof. Tomaž Kosmač

# MENTORING

## Ph. D. Thesis

1. Aljoša Maglica, Innovative electroconductive ceramic composites based on Si3N4 (mentor Tomaž Kosmač; co-mentor Kristoffer Krnel).

# VISITORS FROM ABROAD

- 1. Asst. Prof. Yu Zhang, New York University College of Dentistry, Department of Biomaterials & Biomimetics, Arnold and Marie Schwartz Hall of Dental Sciences, New York, USA, 23-26 June 2011 (lecture: "Development of Graded Glass-Zirconia Restorative Materials")
- Dr. Lars Hälldahl, Mr. S. Nobeta, SPS SYNTEX INC., R & D Center Research & 2. Development Dept., 502 West KSP Kanagawa Science Par, Sakado, Takatsu-ku, Kanagawa, Japonska, 2-8 October 2011

# STAFF

#### Researchers

#### 1. Prof. Tomaž Kosmač, Head

- Asst. Prof. Kristoffer Krnel Postdoctorial associates
- Dr. Aleš Dakskobler 3.
- Dr. Andraž Kocjann 4.
- Dr. Irena Pribošič 5.
- 6 Dr. Krunoslav Vidović\*

#### Postgraduates

- Dr. Aljoša Maglica, left 01.06.11 7.
- 8 Sebastjan Perko, B. Sc.
- 9. Anastasia Samodurova, B. Sc.

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## **ORIGINAL ARTICLES**

- 1. Aleš Dakskobler, Andraž Kocjan, Tomaž Kosmač, "Porous alumina ceramics prepared by hydrolysis-assisted solidification", J. Am. Ceram. Soc., vol. 94, no. 5, pp. 1374-1379, 2011.
- 2. Andraž Kocjan, Aleš Dakskobler, Tomaž Kosmač, "Superhydrophobic nanostructured boehmite coatings prepared by AlN powder hydrolysis", International journal of applied ceramic technology, vol. 8, no. 4, pp. 848-853, 2011.
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## PUBLISHED CONFERENCE PAPERS

#### Regular paper

1. Kostja Makarovič, Janez Holc, Marko Hrovat, Darko Belavič, Marina Santo-Zarnik, Aleš Dakskobler, Andreja Benčan, Marija Kosec, "Biaxial flexural strength of the LTCC material under various firing conditions", In: Proceedings, Goran Stojanović, ed., Milan Radovanović, ed., Novi Sad, University of Novi Sad, Faculty of Technical Sciences, 2011, pp. 81-88.

## 10. Lovro Gorjan\*\*

- 11. Martin Štefanič, B. Sc. **Technical officers**
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Note:

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## PH. D. THESIS

1. Aljoša Maglica, Innovative electroconductive ceramic composites based on Si3N4: doctoral dissertation, Ljubljana, [A. Maglica], 2011.

## PATENT

1. Tomaž Kosmač, Kristoffer Krnel, Andraž Kocjan, Peter Jevnikar, Process for applying adhesion coatings to a substrate, EP2170244 (B1), European Patent Office, 30.3.2011.

## PATENT APPLICATIONS

- 1. Lovro Gorjan, Aleš Dakskobler, Heat treatment process of formed compact using sintering, P-201100196, Urad RS za intelektualno lastnino, 31.5.2011.
- 2. Aljoša Maglica, Kristoffer Krnel, Tomaž Kosmač, Single-stage process of manufacturing a composite ceramic heater, P-201100015, Urad RS za intelektualno lastnino, 13.3.2011.

# 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 the field of intermetallic alloys we continued our research on electrodeposition as a preparation method for nanostructures. Fe-Pd and Co-Pt nanostructures were deposited in high-aspect-ratio alumina or polycarbonate templates. The reactions of Pd and Fe were investigated using cyclovoltametry, where Pd was shown to be irreversible, while Fe deposition was found to overlap with hydrogen evolution. Due to the overall mass-transportlimited deposition, which is characteristic for high-aspect-ratio templates, closely packed Fe<sub>so</sub>Pd<sub>so</sub> nanowires were deposited via pulse plating. Via post-annealing processing, which induced the ordering into the tetragonal phase Head: having high a magnetocrystalline anisotropy, the coercivity was significantly improved up to 120 kA/m. In the Prof. Spomenka Kobe frame of an EU MNT-ERA.Net project, Fe<sub>70</sub>Pd<sub>20</sub> nanotubes and nanowires were successfully synthesised for filtration purposes and in the frame of a national project (together with the National Institute of Chemistry, Slovenia) for the



purposes of targeted drug delivery. The magnetization reversal behaviour in ferromagnetic nanotubes (Fe-Pd and Co-Pt) was investigated using angulardependence measurements and magnetic force microscopy, which showed circumferential magnetization behaviour, which is stable at small applied field angles and coherent rotation stable at higher angles. The magnetization behaviour was also found to depend on the tube-wall thickness, where it was shown that curling is dominant in thin magnetic nanotubes.

We continued with studies on hollow metallic nanoparticles produced by PLD in a nitrogen atmosphere, since this is becoming an area of high potential for future applications in theranostics. These hollow nanospheres were successfully produced from CoPt, Fe, Fe(Sm,Ta) and Al targets.

We have looked at the effects of hydrogen and temperature on the magnetic and structural changes in Nd-Fe-Al alloys with compositions close to Nd<sub>60</sub>Fe<sub>20</sub>Al<sub>10</sub>, using vibrating-sample magnetometry, x-ray diffraction and transmission electron microscopy. At approximately 30 bars and 100°C the material absorbs about 0.6 weight percent of hydrogen. As a result of this hydrogen absorption the coercive field decreases significantly, i.e., from 3750 Oe before to 120 Oe after the hydrogenation. We have used the strong-domainwall-pinning model to explain the coercive field and its drop as a result of the hydrogen absorption. This model can be used to describe the material in the temperature range 250-450 K before hydrogenation for a domain-wall width of 7 nm. After hydrogenation the material displays soft-magnetic behaviour and the possible origins of this are still the subject of our investigations. Our results have demonstrated, once again, the important role that hydrogen can play in modifying the structure and properties of rare-earth-transitionmetal-based permanent-magnet materials.

The grain-boundary diffusion process was used to enhance the coercivity of commercially available Nd-Fe-B sintered magnets. By using electrophoretic deposition (EPD) of DyF<sub>2</sub> or TbF<sub>2</sub> we achieved a spectacular 30% increase in coercivity, without any significant decrease in the remanence. With EPD it is also possible to tailor the coercivities to some extent: by varying the thickness of the coating we are able to tailor the coercivity of the magnet. We successfully performed WDS analyses on Nd-Fe-B magnets doped with Tb (the so-called core-shell structure). The thickness of the Tb-rich shell varied



Figure 1: Necklace formed of hollow, CoPt-based nanospheres: potential application in magnetically and photothermally active nanoparticles for a tuneable drug-delivery and controlled drug-release system.

We have proven and systematically measured the nitrogen gas pressure within individual Albased spheres. The nitrogen pressure ranged between 200 and 600 bars and was generally increasing by decreasing the volume of the void. This is in accordance with the equilibrium gas pressure that would form in a bubble in an Al melt when considering the corresponding surface energy.



Figure 2 A: High-resolution micrograph of the as-cast sample reveals that it is composed of crystalline nanoparticles embedded in a amorphous matrix. (a) According to the SAED pattern, the nanocrystallites are hexagonal neodymium with the following interplanar distances D1=3.116 Å, D2=2.914 Å, D3=2.760 Å, D4=2.126 Å, D5=1.835 Å, D6=1.639 Å (b) EDS of the selected Nd nanoparticles and (c) EDS from a larger area.



Figure 2 B: High-resolution TEM micrograph of the hydrogenated sample reveals that the sample contains more crystalline material and less amorphous matrix than the as-cast sample. (a) SAED reveals that the crystalline particles are the Nd<sub>2</sub>H<sub>2</sub>phase with the corresponding planar distances D1=3.132 Å, D2=2.717 Å, D3=1.916 Å, D4=1.637 Å, D5=1.566 Å and D6=1.356 Å. (b) Enlarged image of the [111] planes in the Nd<sub>2</sub>H<sub>2</sub> nanoparticle. (c) EDS from the Nd<sub>4</sub>H<sub>5</sub>grain.

With a sophisticated thermal treatment we successfully influenced the final microstructure and achieved both goals. If the microstructure is changed in such a way that we get a finely dispersed secondary phase in the magnetocaloric matrix phase, the structural transformation, which is responsible for the high hysteresis losses, occurs at higher magnetic fields. By using low magnetic fields, this effect can be avoided.



Figure 3: The bone grew deeper into the porous titanium layer on the implant surface with a bio-active glass coating (a) than in the case without it (b)

from about 2 µm near the edge of the magnet down to a few tens of nm in its inner part. Quantitative, sub-micrometre-scale EDS and WDS analyses confirmed that upon diffusion the Tb atoms substitute for the Nd atoms in the Nd<sub>2</sub>Fe<sub>14</sub>B matrix phase and the reaction phase  $(Nd_xTb_{1-x})_2Fe_{14}B$  is formed, with the equilibrium Tb concentration being equal to x = 0.5.

We continued our research on the **magnetocaloric effect** of intermetallic alloys and achieved a **breakthrough enhancement of their refrigerating capacity**. Gd<sub>5</sub>Si<sub>2</sub>Ge<sub>2</sub> known as material with a giant magnetocaloric effect has a problem of high hysteresis losses, which has been successfully reduced by adding a fourth element, usually iron, but with the consequence of a reduction of the magnetocaloric effect itself. As a result the refrigerant capacity was only moderately improved. Our goal was to reduce the hysteresis losses and simultaneously keep the high magnetocaloric effect.

In the field of **quasicrystals** we have shown that the tetragonal  $\sigma$ phase and the hexagonal (hex) phase in the Mn-Si-V(Cr) transition-metalalloy systems are stable approximant phases of a dodecagonal (12-fold) quasicrystal that can be prepared in bulk quantities. We have synthesized samples of the  $\sigma$  and *hex* phases of composition Mn<sub>76</sub>Si<sub>18</sub>Cr<sub>6</sub> and determined their magnetic properties. In the  $\sigma$ -Mn<sub>76</sub>Si<sub>18</sub>Cr<sub>6</sub>, a spin-freezing transition to a canonical spin-glass phase was detected below  $T_t \approx 8$  K, characterized by a maximum in the zero-field-cooled susceptibility, a frequency-dependent cusp in the ac susceptibility, M(H) hysteresis, and ultra-slow time decay of the thermo-remanent magnetization. In contrast, no spin-glass transition was observed in the hex- Mn<sub>76</sub>Si<sub>18</sub>Cr<sub>6</sub> phase down to the lowest investigated temperature of 2 K. The analysis of the susceptibility has shown that the coupling of spins in both phases is antiferromagnetic (AFM), but the coupling strength is considerably stronger in the  $\sigma$  phase. In both investigated samples, tiny Mn<sub>2</sub>O<sub>4</sub> inclusions that undergo a transition to a ferrimagnetic phase at  $T_c \approx 42$  K were detected by EDS and in the magnetic signal. The  $\sigma$ phase was obtained by water quenching of the arc-melted precursors, which were heat-treated for 8 days at 1100°C in a sealed silica tube, whereas to get hex phase heat treatment was conducted at 800°C.

The computer modelling was focused on diamond-like carbon (DLC) by performing calculations, that are based on the density-functional theory. A very important application of this study was in tribology, whereas the most important achievement was the investigation of the appearance of magnetism due to the doping with chromium atoms. The experimental results demonstrated the presence of magnetism in chromium-doped, diamond-like carbon. The ab-initio simulations revealed that an external strain due to the substrate is required in order to observe this phenomenon.

In the final year of the Meddelcoat project (FP6, IP-SME), we were mainly engaged in evaluation of the success of the developed **bioactive coatings on metal implants** with a porous surface. In collaboration with the company Helipro d.o.o. we performed extensive metallographic, stereological and histological analysis of the samples tested *in vivo*. Two of the coatings prepared at JSI, i.e., anatase and bioactive glass, revealed a significant enhancement of osseointegration in comparison with the samples without coating or with differently prepared coatings. The research of bioactive glass was also a topic of a bilateral project with the Ruder Bošković Institute in Zagreb, an informal collaboration with Educell d.o.o., as well as of the COST action Namabio that is focused on the development of bioactive scaffolds for stem cells. The titania coatings, in particular their antibacterial properties, remained in our focus via the FP7-ITN project BioTiNet.

In 2011 we strengthened our collaboration with the National Institute for Biology, NIB. The main topic has been a study of **potential health hazard of free titania nanoparticles**, which is lately drawing a lot of attention in the literature. We prepared a comprehensive literature survey (published in J. Radiol.Oncol.) and we collaborated in investigations of their toxicity by characterising various commercial TiO<sub>2</sub> powders. In the journals Nanotoxicology and J. Hazardous Materials we reported that some powders with particles larger than nanosized may also represent a health risk, and in particular UV-irradiated nanoparticles. In addition, an **advantageous cell interaction** with SiC-based ceramics has been also confirmed in collaboration with NIB.

**Perovskite BaTiO**<sub>3</sub> **nanorods** and **SrTiO**<sub>3</sub> **nanotubes** were synthesized via sol-gel electrophoretic deposition into anodic aluminum oxide (AAO) membranes. In the article "Characterization of Individual Barium Titanate Nanorods and Their Assessment as Building-Blocks of New Circuit Architectures" published in Nanotechnology we reported on the integration of individual BaTiO<sub>3</sub> nanorods into simple circuit architectures. Polycrystalline BaTiO<sub>3</sub> nanorods were synthesized by the electrophoretic deposition (EPD) of a barium titanate sol into aluminium oxide (AAO) templates and subsequent annealing. TEM observations revealed the presence of slabs of hexagonal polymorphs intergrown within cubic grains, resulting from the local reducing atmosphere during the thermal treatment. Within the European fusion programme in which we have already collaborated for seven years, the most important result is the optimisation of the SITE-P process developed in our laboratory. The process enables the fabrication of 3-D SiC<sub>f</sub>/ SiC composites for the first-wall blanket in future fusion-power plants. The composite samples analysed at NRG in Petten exhibited high thermal conductivity in the temperature range from 25 °C to 1000 °C that meets the requirement for the material. We also collaborated in other activities of the Slovenian Fusion Association, such as the organisation of the itinerant Fusion Expo and other public-information activities within the European network.

In the field of **photovoltaics** we assembled and tested the DSSC (dye-sensitized solar cells) solar cells. A porous thin film of anatase  $\text{TiO}_2$  on a rigid electrode was prepared by the doctor-blade method. For the manufacturing of the DSSC solar cells on flexible substrates we determined the optimum processing parameters for the preparation of a thin layer of 2-D ordered TiO<sub>2</sub> nanotubes on the Ti foil by anodization of the Ti metal foil.

The use of transparent and conductive films (TCFs) in technologies

of liquid crystal and plasma displays, touch panels, organic light-emitting diodes and solar cells is dominated by indium-tin-oxide (ITO). The high price of In emphasizes the strong need for the development of cheaper alternatives, such as ZnO-based TFSs. Using low-temperature hydrothermal synthesis at 90°C we prepared on the glass substrates, from a water solution of Zn-nitrate and with the addition of Na-citrate, smooth, dense and highly (0001)-oriented polycrystalline ZnO films with an optical transparency of 82% and for undoped films a low resistivity of about 80  $\Omega$ cm. We explained the formation of a highly textured polycrystalline film by a spatially confined oriented growth (SCOG) mechanism, which requires an appropriate nucleation layer on the glass substrate.

Research on oxide thermoelectric materials was focused on the synthesis relative humia of a p-type Ca<sub>3</sub>Co<sub>4</sub>O<sub>9</sub> compound using an alternative approach of mechanochemical alloying. The development and construction of the system for thermoelectric characterization of materials up to 700°C reached its final stage and in the first months of 2012 we are expecting to start with the test measurements.

We started with the development of the **thick-film varistors** on Al<sub>2</sub>O<sub>3</sub> substrates. Inks for screen printing were prepared and the influence of the varistor powder composition on the ink and firing temperature on the formation of the thick film, its interactions with the substrate and its current-voltage (I-U) characteristics were studied.

We continued the study of the synthesis of titania particles in anatase and rutile crystal form using sol-gel and hydrothermal methods. The influence of process parameters on the size, morphology and photocatalytic efficiency of the particles was studied. The nucleation and growth of anatase particles to the specific bi-pyramid morphologies was explained. Due to the difference in the energies of certain crystal planes and the non-equilibrium conditions the growth of starting block-like particles continued through asymmetric rod-like particles, elongated in one of the <101> directions. The particle morphologies were reconstructed from HRTEM images. We continued with a study of the nucleation and crystallization of ZnO nanoparticles to be used as UV absorbers. The crystallization of iron oxide nano-rings was studied by TEM and microanalytical techniques. The self-assembly of Ge quantum dots in an amorphous silica matrix after the high-energy ions' irradiation was investigated using electron microscopy and microanalysis. Together with colleagues from Croatia, Italy and the Czech Republic we published a series of articles explaining self-organization. In collaboration with scientists



Figure 4: (a) Detail of a BaTiO<sub>3</sub> nanorod contacted with FIB nanolithography in a 4-probe configuration. The inset in the upper left corner shows a low-magnification image of the same device. (b) Sensing response of a BaTiO<sub>3</sub> nanorod towards pulses of 100, 50 and 25 % of relative humidity (RH) measured at room temperature. Synthetic air was used as the carrier gas. The inset shows I-V curves obtained in dry and humid (100 % RH) air. A sharp and reversible modulation of the electrical response was observed.

Electrical measurements performed on individual BaTiO<sub>3</sub> nanorods revealed resistivity values between 10 and 100 ohm-cm, which is in good agreement with typical values reported in the past for oxygen-deficient barium titanate films. Consequently, the presence of oxygen vacancies in their structure was indirectly validated. Some of these nanorods were tested as proof-of-concept humidity sensors. They showed reproducible responses towards different moisture concentrations, demonstrating that individual BaTiO<sub>3</sub> nanorods may be integrated in complex circuit architectures with functional capacities.



Figure 5: a) ZnO film on glass prepared by low-temperature hydrothermal synthesis at 90°C from a water solution of Zn-nitrate with the addition of Na-citrate. The inset top-right shows the high optical transparency of the film. b) Schematic presentation of the spatially confined oriented growth (SCOG) mechanism, which in the process of hydrothermal synthesis enables the growth of a dense and highly (0001) textured ZnO film from the nucleation layer on the glass substrate.

In collaboration with the VARSI company two projects were successfully completed. The development of surge protections for solar panels and wind-turbine generators required an improvement to the dc stability of the ZnO-based varistors. Within the project Novel innovative systems for electrical equipment, complexshaped tubular or oval hollow varistors were developed using slip-casting technology.



Figure 6: FEGSEM image of solidified 2- $\mu$ m-sized Au droplet among the Au nano-particles deposited by pulsed-laser deposition - PLD method (F2 laser;  $\lambda = 157 \text{ nm}$ ).

from Portugal the influence of the addition of carbon nano-tubes to  $\text{TiO}_2$  on the **catalytic properties** of the material was studied.

We have investigated the influence of special boundaries in crystal growth. They are known to introduce an abrupt structural and chemical anisotropy, which is readily reflected in an unusual microstructure evolution, whereas their local structure affects the physical properties of polycrystalline materials. These effects can be exploited to tailor the electronic and optical properties of materials. In the non-centrosymmetric structure of ZnO, inversion boundaries (IBs) are the most common type of planar faults that is triggered by the addition of the specific IB-forming dopants (Sb<sub>2</sub>O<sub>2</sub>, SnO<sub>2</sub>, TiO<sub>2</sub>). Their local structure was analysed by conventional TEM techniques and some new methods were developed to resolve their crystallography and atomic-scale chemistry. By knowing the local crystal chemistry of IBs we were able to design experiments to identify their formation mechanism. IBs nucleate in the early stage of grain growth as a dopant-rich topotaxial 2D reaction product on Zn-terminated surfaces of ZnO grains. Soon after their nucleation, ZnO is epitaxially grown on the inherent 2D phase in an inverted orientation, which effectively starts to dictate the anisotropic growth of the infected crystallite. In a very short time the grains with IBs dominate the entire microstructure via an IB-induced exaggerated grain growth mechanism. This phenomenon was used to design the physical properties of ZnO-based varistor ceramics, whereas the bottom-up approach demonstrated here provides the basic tool for the microstructural engineering of functional materials in virtually any system that is prone to the formation of special boundaries.

We studied the twin-boundary formation of Japanese twins in natural quartz. TEM studies confirmed that the twin boundary is in accordance with the Japan twin law; however, the appearance of the boundary is changing rapidly across the twinned crystal, suggesting that the twin formation is associated only with the early nucleation stage of the crystal growth.

For the reliable characterization of various materials on the micro- and nanometre scales we have applied advanced methods of high-resolution scanning electron microscopy (FEGSEM) and energy-dispersive and wavelengthdispersive X-ray spectroscopies, EDS and WDS.

Using these methods we have characterized the morphology and the chemical composition of various nano-materials, such as FePd and CoPt nanorods and thin films, TiO<sub>2</sub> and ZnO nanoparticles and submicrometersized reaction phases in the Nd-Fe-B sintered magnets doped with Tb. The obtained results allowed us to explain the influence of the process parameters of production and/or the modification of the investigated materials on their physical and chemical properties.

In the field of analytical electron microscopy we were also involved in establishing the TEM analytical procedure for reliable, quantitative compositional analysis of perovskite ceramics that contain volatile alkaline compounds. To discriminate the material-specific composition from the artefacts introduced during the EDXS/TEM analyses, the effects of radiation damage

and the absorption of the characteristic X-ray lines were studied in detail by combined EDXS and EELS analysis. One of the important research areas of the group is the implementation and development of various electron microscopy analytical techniques within the existing EU project ESTEEM, such as electron energy-loss spectroscopy

(EELS), high-resolution scanning transmission electron microscopy (STEM, HAADF-STEM) electron holography and the mechanical preparation of the TEM samples. The research group is additionally strongly involved in managing of the Center for Electron Microscopy within the frame of the national infrastructure Center for Microstructural and Surface Analysis. The implementation of various electron microscopy analytical techniques and the possibility for researchers to access the research infrastructure for electron microscopy is of utmost importance for numerous research institutions,

EDS and WDS methods were optimized and improved for the nanometre-scale compositional analyses by the implementation of lowvoltage microscopy and X-ray spectroscopic measurements of low-energy spectral lines with energies below 5 keV. industrial partners (Cinkarna Celje, SwatyComet, Hidria AET, Iskra Zaščite, Termoelektrarna Toplarna Ljubljana, ITW Metalflex, ZZZV Maribor, Kolektor), as well as for graduate and post-graduate education.

## Some outstanding publications in the past year

- 1. S. Kobe, B. Podmiljšak, P. J. McGuiness and M. Komelj, CMAs as magnetocaloric materials, a chapter in the book Complex Metallic Aalloys: Fundamentals and Applications, Weinheim: Wiley-VCH, 2011
- K. Žagar, F. Hernandez-Ramirez, J. D. Prades, J.R. Morante, A. Rečnik and M. Čeh. Characterization of individual barium titanate nanorods and their assessment as building blocks of new circuit architectures. *Nanotechnology* (*Bristol*), 2011, vol. 22, no. 38, str. 385501-1-385501-6.
- A. Ivekovič, G. Dražić, S. Novak, Densification of a SiC-matrix by electrophoretic deposition and polymer infiltration and pyrolysis process. *J. Eur. Ceram. Soc.*. [Print ed.], 2011, vol. 31, no. 5, str. 833-840, doi: 10.1016/j. jeurceramsoc.2010.11.021.
- N. Daneu, A. Rečnik, S. Bernik, Grain-growth phenomena in ZnO ceramics in the presence of inversion boundaries, J. Am. Ceram. Soc., 94 (5), (2011), 1619-1626
- K. Žužek Rožman, D. Pečko, L. Suhodolčan, P.J. McGuiness, S. Kobe, Electrochemical syntheses of soft and hard magnetic Fe<sub>50</sub>Pd<sub>50</sub>-based nanotubes and their magnetic characterization. *J. alloys compd.*. [Print ed.], 2011, vol. 509, issue 2, str. 551-555, doi: 10.1016/j.jallcom.2010.09.108.
- A. Kocjan, S. Kovačič, A. Gradišek, J. Kovač, P.J. McGuiness, T. Apih, J. Dolinšek, S. Kobe, Selective hydrogenation of Ti-Zr-Ni alloys. *Int. j. hydrogen energy*. [Print ed.], 2011, vol. 36, issue 4, str. 3056-3061, doi: 10.1016/j. ijhydene.2010.11.116.

## Patents granted

- 1. Bioactive and photocatalytic coating on metal implants and a process of preparing thereof Saša Novak, Nataša Drnovšek
  - SI23312 (A), Slovenian Intelectual Property Office, 19 March 2011.
- Anatase nanoparticles and procedure for synthesis of anatase nanoparticles Dejan Verhovšek, Tomi Gominšek, Miran Čeh, Pavel Blagotinšek, Sašo Šturm, Kristina Žagar SI23219 (A), Slovenian Intelectual Property Office, 31 May 2011.
- Rutile nanoparticles and procedure for synthesis of rutile nanoparticles Dejan Verhovšek, Tatjana Rožman, Miran Čeh, Pavel Blagotinšek, Sašo Šturm, Kristina Žagar SI23218 (A), Slovenian Intelectual Property Office, 31 May 2011.

Improved magnetocaloric material and procedure of its manufacture Benjamin Podmiljšak, Paul John McGuiness, Spomenka Kobe SI23405 (A), Slovenian Intelectual Property Office, 30 December 2011.

## Awards and appointments

- Medeja Gec, Tea Toplišek, Goran Dražić: "Preparation of Sigma<sup>™</sup> SiC fibres for TEM by tripod polishing and conventional ion milling"; a Poster Award for the best poster in Instrumentation and Methodology, MCM2011 - 10<sup>th</sup> Multinational Congress on Microscopy 2011, Urbino, Italy, 4–9 September 2011
- Zoran Samardžija & Darko Makovec: "EPMA-WDS quantitative compositional analysis of barium titanate ceramics doped with cerium"; The Best Poster Award at the 12<sup>th</sup> European Workshop on Modern Developments and Applications in Microbeam Analysis – EMAS 2011, Angers, France, 15–19 May 2011
- 3. Marko Soderžnik, Paul McGuiness, Kristina Žužek Rožman, Spomenka Kobe: The best presentation among young researchers in the research field Nanomaterials and Nanotechnology, 19<sup>th</sup> Conference on Materials and Technology, Portorož, Slovenia, 22–23 November 2011. The title of the awarded presentation: Electrophoretic Deposition of DyF<sub>3</sub> on Nd-Fe-B Sintered Magnets

## Organization of conferences, congress and meetings

- 1. 1st BioTiNet Workshop »Advanced Methods for Materials Characterization«, Ljubljana, Slovenia, 23–27 October 2011
- Čím budú svietiť deti vašich detí, Fusion Maxi EXPO, Avion Shopping Park, Bratislava, Slovak Republic, 5 January – 18 February 2011 (co-organisation)
- 3. Fusion Energiequelle der Zukunft, Fusion EXPO Maxi, TU Wien, Vienna, Prechtlsaal, Austria, 1–10 March 2011 (co-organisation)

- 4. Énergie Fusion, Énergie du futur, Fusion EXPO Maxi, Palais de la musique et des congrès Pierre-Pflimlin, Strasbourg, France, 26 June 2 July 2011 (co-organisation)
- 5. Fusion Expo at the Lowlands Music Festival 2011, Biddinghuizen, The Netherlands, 19–21 August 2011 (coorganisation)
- Fusion show "Plasma's. Fusie! Energie?", Campus Drie Eiken, Antwerpen (Wilrijk), Belgum, 17–23 November 2011 (co-organisation)
- 7. 19th Conference on Materials and Technologies, Portorož, Slovenia, 22-23 November 2011 (co-organisation)
- 8. 10<sup>th</sup> Multinational Congress on Microscopy 2011 MCM2011, Urbino, Italy, 5–9 September 2011 (membership in International Advisory Board)
- 9. C-MAC Days 2011, University of Liverpool, Liverpool, United Kingdom, 8–9 November 2011 (membership in Science Board and General Assembly in the European Integrated Center for the Development of New Metallic Alloys and Compounds (C-MAC))

# INTERNATIONAL PROJECTS

- Academic-Industrial Initial Training Network on Innovative Biocompatible Titaniumbase Structures for Orthopaedics BioTiNet 7. FP, 264635 FUSEX EC; Prof. Jürgen Eckert, Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany Prof. Spomenka Kobe, Asst. Prof. Saša Novak Krmpotič 2. Tailoring of Tribological Interfaces for Clean and Energy-Efficient Diesel and Gasoline Power Trains 2020 INTERFACE 7. FP, 234324, SCP8-GA-2009-234324 EC, Jacqueline Kidd, PA - Support Officer to Director of Research, Institute of Engineering Thermofluids, Surfaces and Interfaces, School of Mechanical Engineering, The University of Leeds, Leeds, Great Britain Asst, Prof. Matei Komeli Merging Atomistic and Continuum Analysis of Nanometer Length-scale Metal-oxide 3. 12 Systems for Energy and Catalysis Applications MACAN 7. FP, 233484, NMP3-CA-2009-233484 EC; Prof. Wayne Kaplan, Technion - Israel Institute of Technology, Haifa, Israel Asst. Prof. Aleksander Rečnik 4. Improving the Gender Diversity Management in Materials Research Institutions DIVERSITY 7. FP, 230253 EC; Dr. Oliver Gutfleisch, Leibniz-Institut für Festkörper- und Werkstoffforschung, ESTEEM Dresden, Germany 6. FP, 026019 Prof. Spomenka Kobe 5. Cooperation of Space NCPs as a Means to Optimise Services COSMOS 14. 7. FP, 218813 Hy-nano-IM EC; Dr. Adrien Klein, Deutsches Zentrum für Luft und Raumfahrt e.v., (DLR), Köln, Germany Prof. Spomenka Kobe, Dr. Boris Pukl, Dr. Špela Stres 15. Production of a Dense SIC-based Composite with Closed Porosity - 4.1.1.1 - FU NSFM EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association - SFA 3211-08-000102, FU07-CT-2007-00065 EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Goran Dražič Optimisation of Thermal Conductivity of SIC Composite - 4.1.1.1. 7. WP11-MAT-SiC/SiC-02-01/PS EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association - SFA 17. 3211-08-000102, FU07-CT-2007-00065 EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Goran Dražič, Asst. Prof. Saša Novak Krmpotič 8 Definition of a Fabrication Route for an Optimised SiC-based Composite - 4.1.1.2. WP11-MAT-SiC/SiC-01-01-PS/MHEST EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association – SFA 3211-08-000102, FU07-CT-2007-00065 EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Saša Novak Krmpotič 9 Review R&D on Materials - 4.1.1.2 WP11-DAS-MAT-M03-01/MHEST/PS EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association - SFA 3211-08-000102, FU07-CT-2007-00065 BI-CN/09-11-009
- EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Saša Novak Krmpotič 10. Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN-EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association - SFA 3211-08-000102, FU07-CT-2007-00065 EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Saša Novak Krmpotič, Tomaž Skobe, B. Sc., Melita Lenošek Kavčič, B. Sc., Asst. Prof. Igor Lengar 11. Public Information; Research Unit - Administration and Services - RU-FU EURATOM - MHEST 7. FP - EURATOM, Slovenian Fusion Association – SFA Annex 3, 3211-08-000102, FU07-CT-2007-00065 EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Asst. Prof. Saša Novak Krmpotič, Prof. Milan Čerček Multifunctional Bioresorbable Biocompatible Coatings with Biofilm Inhibition and Optimal Implant Fixation 6. FP, MEDDELCOAT NMP3-CT-2006-026501 EC; Prof. Jozef Vleugels, Katholieke Universiteit Leuven, Research & Development, Leuven, Belgium Asst. Prof. Saša Novak Krmpotič 13. Distributed European Infrastructure of Advanced Electron Microscopy for Nanoscience EC; Prof. Gustaaf Van Tendeloo, Universiteit Antwerpen, Antwerpen, Belgium Prof. Miran Čeh, Asst. Prof. Sašo Šturm Hydrogen Impermeable Nano-material Coatings for Steels MNT ERA NET Asst. Prof. Paul McGuiness Novel Smart Filtration Media MNT-ERA-NET II Warsaw University of Technology (WUT), Warsaw, Poland Dr. Kristina Žužek Rožman 16. From Nano to Macro Biomaterials (Design, Processing, Characterization, Modelling) and Applications to Stem Cells Regenerative Orthopedic and Dental Medicine COST MP1005, NAMABIO EC; COST Office, Brussels, Belgium Asst. Prof. Saša Novak Krmpotič, Nataša Drnovšek, B. Sc. Investigation of Electrical Mobility and Dielectric Relaxation of Bioactive Glass BI-HR/10-11-002 Dr. Andrea Moguš-Milanković, Ruđer Bošković Institute, Zagreb, Croatia Asst. Prof. Saša Novak Krmpotič Correlation of Structure and Properties of Nanostructured Perovskites BI-HR/10-11-027 Dr. Andreja Gajović, Ruđer Bošković Institute, Zagreb, Croatia Asst. Prof. Sašo Šturm Advanced Methods and Technologies for Processing of a New Generation of ZnO-based Varistor Ceramics BI-CN/09-11-017 Dr. Zheng Liaoying, The Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China Asst. Prof. Slavko Bernik 20. Novel Magnetocaloric Materials for Ecological Refrigeration

Dr. Yan Gaolin, School of Physics and Technology, Wuhan University, Wuhan, China Asst. Prof. Paul McGuiness

21. Nanofabrication and Advanced Characterization of Funtionalised Materials  $BI\mbox{-}PT/10\mbox{-}11\mbox{-}009$ 

Dr. Adrian M. T. Silva, Laboratory of Catalaysis and Materials, Faculty of Engineering, University of Porto, Porto, Portugal Asst. Prof. Goran Dražić

22. Electron Energy-Loss Spectroscopy of Boron Incorporation in Strontion Aluminate BI-TR/11-13-007

Asst. Prof. Cleva Ow-Yang-Gülgün, Sabanci University, Faculty of Engineering and Natural Science, Tuzla, Istanbul, Turkey Asst. Prof. Sašo Šturm

23. Investigation of High Temperature Reactions between Doped Perovskite Components in a Solid Oxide Fuel Cell

BI-TR/10-12-005 Asst. Prof. Mehmet Ali Gülgün, Sabanci University, Faculty of Engineering and Natural Science, Tuzla, Istanbul, Turkey Prof. Miran Čeh

# R & D GRANTS AND CONTRACTS

- 1. New metallic materials for thermal storage of digital information Dr. Andraž Kocjan
- 2. Twinning, epitaxy and phase transformations in minerals Asst. Prof. Nina Daneu
- Near-net shape nanoparticle-reinforced polymer-composites for highly-loaded advanced mechanical components with superior tribological performance Asst. Prof. Saša Novak Krmpotič
- Electron microscopy and microanalysis of materials on submicrometer scale Dr. Zoran Samardžija
- Hydrothermal synthesis of strongly adhered TiO<sub>2</sub> photocatalytic coatings on metallic substrates
- Asst. Prof. Goran Dražić
- Novel functionalized nanomaterials for applications as nano- or biosensors/actuators/ bioresponsive (carrier) systems Dr. Kristina Žužek Rožman
- 7. Exploration and preservation of mineralogical heritage
- Asst. Prof. Aleksander Rečnik 8. Microbial adhesion management on material surfaces
- Asst. Prof. Goran Dražić
- 9. Physics and chemistry of interfaces of nanostructured metallic materials Prof. Miran Čeh
- 10. High-coercivity Nd-Fe-B bonded magnets for automotive applications Prof. Spomenka Kobe

- 11. Protected Permanent Magnets for Advanced High-Temperature Applications Asst. Prof. Paul John Mcguiness
- Materials and technologies for applications of ZnO-based thick-film varistors and oxide thermoelectrics Asst. Prof. Slavko Bernik
- Colour, absorption and protective nanolayer coatings for aluminium alloy Prof. Dr. Miran Čeh (Dr. Peter Panjan)
- 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 TiO<sub>2</sub> nanoparticle surface: prevention of agglomeration and preservation of intrinsic properties Asst. Prof. Aleksander Rečnik
- Innovative production systems for vaccines and regenerative medicine Asst. Prof. Aleksander Rečnik

# **RESEARCH PROGRAM**

1. Nanostructured materials Prof. Spomenka Kobe

# NEW CONTRACTS

- High-coercivity Nd-Fe-B bonded magnets for automotive applications Kolektor Group, Vodenje in upravljanje družb d.o.o., Idrija Prof. Spomenka Kobe
- Protected permanent magnets for advanced high-temperature applications MAGNETI, Ljubljana, Podjetje za proizvodnjo magnetnih materialov, d.d., Ljubljana Asst. Prof. Paul McGuiness
- 3. Materials and technologies for applications of ZnO-based thick film varistors and oxide thermoelectrics
- VARSI, podjetje za proizvodnjo varistorjev in sklopov, d.o.o., Ljubljana Asst. Prof. Slavko Bernik
- Materials and technologies for applications of ZnO-based thick film varistors and oxide thermoelectrics
- KEKON keramični kondenzatorji, d.o.o., Žužemberk Asst. Prof. Slavko Bernik
- 5. Nano varistor RC eNeM Nanovaristor, Ljubljana Asst. Prof. Slavko Bernik

# MENTORING

## Ph. D. Theses

- Katja König, The production of advanced ceramic materials by electrophoretic deposition (mentor Spomenka Kobe; co-mentors Saša Novak Krmpotić, Aldo R. Boccaccini).
- 2. Tea Toplišek, Ceramic composites with long silicon-carbide fibers (mentor Spomenka Kobe).
- 3. Kristina Žagar, Synthesis and characterization of perovskite nanostructures (mentor Miran Čeh).

## Bologna M. Sc. Thesis

 Milena Zorko, Self-assembled structures based on monodisperse spherical silica particles (mentor Saša Novak Krmpotič; co-mentor Miran Gaberšček).

# VISITORS FROM ABROAD

- Dr Velimir Radmilović, National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, University of California, Berkeley, USA, 20–21 January 2011
- Dr Mehmet Ali Gülgün, Shalima Shawuti and Gulcan Corapcioglu, Sabanci University, Istanbul, Turkey, 17–24 February 2011

- Prof. A. C. Cefalas, National Hellenic Research Foundation HNRF, Athens, Greece, 17–19 February 2011
- Dr Ulrike Wolf, Leibniz-Institut f
  ür Festkörper- und Werkstoffforschung IFW, Dresden, Germany, 27 March – 15 April 2011
- Prof. Norberto Roveri, Martina Lorenzetti, Alma Mater Studiorum, Università di Bologna, Lab. LEBSC, Bologna, Italy, 7-9 March 2011
- 6. Dr Aguar Pilar, European Commission, DG Research, Brusells, Belgum; Prof. Jef Vleugels, Prof. Omer Van Der Biest, Tina Mattheys, Annabel Braem, Bram Neirinck, Katholieke Universiteit Leuven, MTM, Leuven, Belgium; Prof. Jozef Anné and Lieve Van Mellaert, Katholieke Universiteit Leuven, CEMOL, Leuven, Belgium; Marko Gradišar, HELI PRO d. o. o., Lesce, Slovenia; Prof. Monika Willert-Porada and Dr Andreas Rosin, Universität Bayreuth, Bayreuth, Germany; Dr Martie-Françoise Harmand, Laboratoire d'Evaluation des Matériels Implantables LEMI, Martillac, France; Jordi Garcia-Forgas, Peyer Fertigungstechnik AG, Waltenschwil, Switzerland; Dr Martin Erdtmann, HEMOTEQ GmbH, Würselen, Germany; Dr Paul Michelis, Institute of Mechanics of Materials and Geostructures IMMG SA, Penteli, Greece; Prof. Michael Gasik, Helsinki University of Technology HUT, Espoo, Finland; Dr Alessandro Facchini and Dr Michele Pressacco, LIMA-LTO S.P.A., Udine, Italy; Dario Pirovano, EUCOMED, Woluwe St. Pierre, Belgium; Matevž Gorenšek, EDUCELL, d.o.o., Ljubljana, Slovenia; 14–15 March 2011
- 7. Dr Andreja Gajović, Rudjer Bošković Institute, Zagreb, Croatia, 5–8 April 2011
- Katarzyna Kwapiszewska, Politechnika Warszawska, Warsaw, Poland, 1 July 25 August 2011
- Prof. Francisco Hernández-Ramírez, Institut de Recerca en Energia de Catalunya IREC, Barcelona, Spain, 3–4 May 2011
- Muhammad Shahid Arshad, Royal Institute of Technology KTH, Stockholm, Sweeden, 16–20 May 2011
- 11. Dr Maxime Feraille, Embassy of Republic of France, Ljubljana, Prof. Janez Kranjc, Faculty of Law, University of Ljubljana, Slovenia, 23 May 2011

# Jožef Stefan Institute

- Dr Mehmet Ali Gülgün, Dr Cleva Ow-Yang, Melike Mercan Yildizhan, Gulcan Corapcioglu and Guliz Inan, Sabanci University, Istanbul, Turkey, 7–14 August 2011
- Milivoj Plodinec, Dipl. Eng. Phys., Institut Ruđer Bošković, Zagreb, Croatia, 15 October - 15 April 2012
- 14. Dr Jakub Michalski, Dr Wojciech Fabianowski, Politechnika Warszawska, Warsaw, Poland; Prof. Wojciech Piątkiewicz, Polymem, Warsaw, Poland; Prof. Leon Gradoń, SecuraNova, Warsaw, Poland; Dr Iztok Naglič, Faculty of Natural Sciences, University of Ljubljana, Slovenia; Marko Tandler, Litostroj Jeklo, Ljubljana, Slovenia, 29–30 September 2011
- Dr Cheng Lihong, Shanghai Institute of Ceramics, Chinese Academy of Science, Shanghai, China, 22 September – 30 November 2011

# STAFF

#### Researchers

- 1. Asst. Prof. Slavko Bernik
- 2. Prof. Miran Čeh
- 3. Asst. Prof. Nina Daneu
- 4. Asst. Prof. Goran Dražić
- 5. Prof. Spomenka Kobe, Head
- 6. Asst. Prof. Matej Andrej Komelj
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- 14. Dr. Benjamin Podmiljšak
- 15. Dr. Kristina Žagar
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- 17. Sandra Drev, B. Sc.
- 18. Nataša Drnovšek, B. Sc.
- Ana Gantar, B. Sc.
   Barbara Horvat, B. Sc.

- 16. Radovan Bolko, Igor Draksler, Ludvik Kumar, Dr Boris Saje, Kolektor Group, Idrija, Slovenia, 14 November 2011
- 17. Dr Andreja Gajović, Rudjer Bošković Institute, Zagreb, Croatia, 14–18 November 2011
- Dr Luisa Maria Pastrana Martinez, FEUP Faculdade de Engenharia da Universidade do Porto, Porto, Portugal, 20–27 November 2011
- 9. Prof. Jean-Marie Dubois, Jean Lamour Institute, Nancy, France, 7–8 December 2011
- Ricardo Segundo, FEUP Faculdade de Engenharia da Universidade do Porto, Porto, Portugal, 26–30 December 2011
- 21. Dr Andreja Gajović, Rudjer Bošković Institute, Zagreb, Croatia, 26-30 December 2011
- 21. Aljaž Iveković, B. Sc.
- 22. Marja Jerič, B. Sc.
- 23. Dr. Katja König, left 15.12.11
- 24. Mateja Košir, B. Sc.
- Matic Krivec, B. Sc.
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- 27. Martina Lorenzetti, M. Sc.
- 28. Darja Pečko, B. Sc.
- 29. Matejka Podlogar, B. Sc.
- 30. Mojca Presečnik, B. Sc.
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- 39. Medeja Gec, B. Sc.

Note: \*\* postgraduate financed by industry

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## **ORIGINAL ARTICLES**

- 1. Marcela Achimovičová, Peter Baláž, Juraj Ďurišin, Nina Daneu, Juraj Kováč, Alexander Šatka, Armin Feldhoff, Eberhard Gock, "Mechanochemical synthesis of nanocrystalline lead selenide: industrial approach", *Int. j. mater. res.*, vol. 102, no. 4, pp. 441-445, 2011.
- Marcela Achimovičová, Klebson Lucenildo da Silva, Nina Daneu, Aleksander Rečnik, Sylvio Indris, Holger Hain, Marco Scheuermann, Horst Hahn, Vladimir Šepelák, "Structural and morphological study of mechanochemically synthesized tin diselenide", *J. mater. chem.*, vol. 21, issue 16, pp. 5873-5876, 2011.
- Slavko Bernik, Matejka Podlogar, Nina Daneu, Aleksander Rečnik, "A novel approach to tailoring the microstructure and electrical characteristics of ZnO-based varistor ceramics via inversion-boundary (IB) induced grain growth", *Zašt. mater.*, vol. 52, no. 2, pp. 73-79, 2011.
- 4. Maja Buljan, I. Bogdanović-Radović, M. Karlušić, Uroš Desnica, Nikola Radić, Milko Jakšić, K. Salomon, Goran Dražić, Sigrid Bernstorff, Václav Holý, "Design of quantum dot lattices in amorphous matrices by ion beam irradiation", *Phys. rev., B, Condens. matter mater. phys.*, vol. 84, no. 15, pp. 155312-1-155312-8, 2011.
- 5. Jui Chakraborty, Nina Daneu, Aleksander Rečnik, Manjusha Chakraborty, Sudip Dasgupta, Jiten Ghosh, Somoshree Sengupta, Sujuta Mazumdar, Mithlesh Sinha, Debabrata Basu, "Stepwise formation of crystalline apatite in the biomimetic coating of surgical grade SS 316L substrate: a TEM analysis", *Journal of the Taiwan institute of chemical engineers*, vol. 42, no. 4, pp. 682-687, 2011.

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- 7. Nina Daneu, Aleksander Rečnik, Slavko Bernik, "Grain-growth phenomena in ZnO ceramics in the presence of inversion boundaries", *J. Am. Ceram. Soc.*, vol. 94, no. 5, pp. 1619-1626, 2011.
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- 9. X. Gao, Hui Gu, Y. -X. Li, Z.-G. Yi, Miran Čeh, Kristina Žagar, "Structural evolution of the intergrowth bismuth-layered Bi<sub>7</sub>Ti<sub>4</sub>NbO<sub>21</sub>", *J. Mater. Sci.*, vol. 46, no. 16, pp. 5423-5431, 2011.
- Helder T. Gomes, Bruno Machado, Adrián M. T. Silva, Goran Dražić, Joaquim Luís Faria, "Photodeposition of Pt nanoparticles on TiO<sub>2</sub>carbon xerogel composites", *Mater. lett.*, vol. 65, no. 6, pp. 966-969, 2011.
- 11. Marijan Gotić, Goran Dražić, Svetozar Musić, "Hydrothermal synthesis of [alpa]-Fe[sub]20[sub]3 nanorings with the help of divalent metal cations, Mn<sub>2+</sub>, Cu<sub>2+</sub>, Zn<sub>2+</sub> and Ni<sub>2+</sub>,", In: Proceedings of the EUCMOS 2010, 30th European Congress on Molecular Spectroscopy, Florence, Italy, *J. Mol. Struct.*, vol. 993, no. 1/3, 2011.
- Aljaž Iveković, Goran Dražić, Saša Novak, "Densification of a SiC-matrix by electrophoretic deposition and polymer infiltration and pyrolysis process", J. Eur. Ceram. Soc., vol. 31, no. 5, pp. 833-840, 2011.
- 13. S. Kashimoto, Andraž Kocjan, Zvonko Jagličić, Simon Jazbec, H. Iga, T. Ishimasa, Janez Dolinšek, "Magnetic properties of  $\sigma$  and hexagonal-Mn <sub>76</sub>Si <sub>18</sub>Cr <sub>6</sub> approximant phases of a dodecagonal quasicrystal",

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- 15. Andraž Kocjan, Paul J. McGuiness, Spomenka Kobe, "The impact of ambient gas on the magnetic properties of Ti<sub>40</sub>Zr<sub>40</sub>Ni<sub>20</sub> powders during mechanical alloying", *J. magn. magn. mater.*, vol. 323, issue 3-4, pp. 301-305, 2011.
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Clinoptilolite from Serbia", *Clays and clay miner.*, vol. 59, no. 3, pp. 277-285, 2011.

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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 2010 our investigations were 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 of magnetic nanoparticles has mainly been focused on bonding different biologically-active molecules to the surfaces of functionalized superparamagnetic iron oxide maghemite nanoparticles. The nanoparticles were functionalized by bonding different organosilane molecules to their surfaces, usually through a thin surface layer of silica. The functionalization molecules provide specific functional groups for the further bonding of biologically-active molecules to the nanoparticles' surfaces. At the same time, the functionalization layer allows the nanoparticles compatibility with physiological fluids and prevents their agglomeration. Different (bio)molecules were bonded onto the nanoparticles for their potential use in biomedicine. The main focus was on bonding target-

ing ligands, which enable the targeted delivery of the nanoparticles in cancer cells. In cooperation with the Department for Biotechnology, JSI, and the Faculty of Pharmacy, Ljubljana, we studied nanoparticles' targeting into cancer cells using the bonding of epidermal growth factor (EGF) molecules onto the functionalized nanoparticles. EGF molecules recognize specific receptors, which are over-expressed at the cancer cells. The focus was on the influence of the type of the EGF bonding on the targeting efficiency.

We have continued to study the hydrothermal nanoparticles synthesis of barium hexaferrite and strontium hexaferrite ( $BaFe_{12}O_{19}$ ,  $SrFe_{12}O_{19}$ ). Up to now, we managed

to synthesize ultrafine hexaferrite nanoparticles of discoid shape, approximately 10 nm wide, but only over 3 nm thick. In cooperation with colleagues from the Department for Low and Intermediate Energy Physics and from the Department of Nanostructured Materials, JSI, we systematically studied their structural properties using x-ray diffractometry (XRD), quantitative high-resolution electron microscopy (HREM), x-ray absorption spectroscopy

(EXAFS) and Mössbauer spectroscopy (MS). The nanoparticles display structural and magnetic properties much different to those of the bulk, mainly due to their very small thickness compared to the size of a unit cell of their hexagonal structure. For the majority of applications, somewhat larger nanoparticles would be of interest. However, the synthesis method did not enable the control of their size. Namely, the ultrafine nanoparticles are only obtained at low temperatures of the hydrothermal treatment, just above the formation temperature of the hexaferrite, where Ostwald ripening is not yet active. The primary growth of the nanoparticles at low temperatures is very limited, whereas at higher temperatures the growth by Ostwald ripening is too fast to be controlled. To control the nanoparticle size, the influence of different surfactants on their growth was studied. It appeared that the surfactant oleic acid completely blocks the growth across a broad temperature region, whereas carboxymethyl cellulose only partially impedes the growth. Using the addition of the surfactant carboxymethyl cellulose we managed to synthesize hexaferrite nanoparticles with a size of 20 nm, which displayed satisfactory magnetic properties.

One part of the research was devoted to the hydrothermal synthesis of the magnetic perovskite LaSrMnO<sub>3</sub>. Chemical reactions taking place during the hydrothermal treatment of an aqueous suspension of constituting-cation hydroxides were systematically studied. It appeared that two solid solutions are formed at temperatures above 240 °C: a perovskite solid solution La<sub>1</sub>

The influence of different types of bonding of the targeting ligand, epidermal growth factor onto the magnetic particles on their targeted delivery in specific cancer cells was studied *in vitro*.



nalization layer allows the *Prof. Darko Makovec* . Different (bio)molecules cus was on bonding target-

300 nm

 $_{x}$ Sr $_{x}$ MnO $_{3}$  and a solid solution Sr $_{1x}$ La $_{x}$ MnO $_{3}$  with the hexagonal perovskite structure. The formation of the perovskite is favoured when the hydroxides are precipitated in an inert atmosphere, preventing the oxidation of Mn<sup>2+</sup>. In this

The structural properties of ultrafine nanoparticles of barium hexaferrite were studied. in the shape of hexagonal platelets similar to snowflakes. The synthesis of cobalt ferrite ( $CoFe_2O_4$ ) nanoparticles by co-precipitation and the hydrothermal method was also investigated. Both methods are suitable for the synthesis

case, the perovskite phase grows as dendrites with a specific shape of "pine trees" or

of spinel ferrite nanoparticles in the size region from sizes where superparamagnetism dominates to the region where ferrimagnetism dominates the magnetic properties. The influence of synthesis conditions on the formation and growth of the nanoparticles was systematically investigated. To get a better insight into the formation mechanism, the potentiometric titrations of the Fe<sup>3+</sup> and Co<sup>2+</sup> solutions were conducted at room temperature. Both cations precipitate at markedly different pH values. Therefore, a dissolution and re-crystallization mechanism was proposed for the formation of the cobalt ferrite nanoparticles. For certain applications, colloidal suspensions of ferrimagnetic nanoparticles in non-polar liquids are desired. Because oleic acid is normally used as the surfactant, all of the syntheses were conducted in the presence of oleic acid. The oleic acid interferes with the



Figure 2: Dendrites of magnetic perovskite LaSrMnO3.

formation and growth of the cobalt ferrite nanoparticles. Namely, the formation temperature of the spinel phase was increased and the particle growth was limited. Because the particles growth was limited, the relatively high synthesis temperature could be applied and the synthesized nanoparticles were ferrimagnetic, yet small enough that their colloidal suspensions can be prepared.

 $CoFe_2O_4$  shows magnetic properties that are not typical for spinel ferrites, i.e. high magnetic anisotropy, which results in high coercivity and magnetostriction. It shows the largest magnetostriction among oxide materials and is therefore suitable for the application in multifunctional composites like: magneto-optic elements, which have been developed in the frame of an international project FOMS (see below), or in magneto-dielectrics, in which the 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 possibility of assembling  $CoFe_2O_4$  nanoparticles into organized microstructures under an applied magnetic field. Stable suspensions from particles of various sizes and magnetic properties were deposited on corundum substrates and dried in magnetic fields of different strengths. The homogeneity of the deposits increases with the decreasing magnetiza-

tion and coercivity of the nanoparticles, as well as with the decreasing strength of the applied magnetic field. The agglomeration of particles increases due to the magnetic dipole-dipole interaction with the improvement of the nanoparticles' magnetic properties and/or increasing magnetic field. Finally, nanoparticles assemble into micron-or millimetre-sized columns. 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. A large part of our research was devoted to the coating of thin layers of magnetic iron oxide onto different sub-

strates using simple precipitation from the aqueous solutions. The coating of magnetic layers is especially interesting

as a tool for the synthesis of nanocomposite particles composed of a core of specific functional material and a magnetic shell. Here, our research was mainly focused in the synthesis of nanocomposite particles composed of a hard-magnetic hexaferrite core and the soft-magnetic maghemite shell. Such nanocomposite particles would display an optimal shape of their magnetic hysteresis for use in magnetic hyperthermia. The coating is formed by the heterogeneous nucleation of iron (oxy)hydroxide at the surfaces of the core particles during the precipitation of Fe<sup>2+</sup>/Fe<sup>3+</sup> ions. To enable the heterogeneous nucleation, the kinetics of the chemical reactions and consequently the supersaturation of the products in the solution have to be closely controlled. The

control of supersaturation was possible if the hydroxyl ions and  $Fe^{3+}$  ions were slowly released: the first during the dissolution of Mg(OH)<sub>2</sub> and the second during the decomposition of the Fe-urea complex. Subsequently, the formed layer of iron (oxy)hydroxide at the surfaces of the core particles transforms into the magnetic maghemite. When the layer was coated onto the barium-hexaferrite core particles, the maghemite grew epitaxially on the structurally similar hexaferriate with spinel {111} planes parallel to the hexaferrite basal {0001} planes.

An important new area of research was devoted to materials for magnetic separation. For magnetic separation, different molecules/biomolecules/cells are specifically bonded to the magnetic carriers, which enable their

A new method of coating thin layers of magnetic iron oxides using the simple precipitation of iron ions from their aqueous solutions enabled the synthesis of nanocomposite particles composed of a hard-magnetic Ba-hexaferrite core and a soft-magnetic maghemite shell. separation from the mixture using an external magnetic field. Frequently, superparamagnetic nanoparticles are considered as the magnetic carriers; however, they are actually inefficient in industrial applications. Namely, the

force acting on the nanoparticle in the magnetic-field gradient is too weak for their efficient magnetic separation. For efficient separation, the magnetic carriers have to be superparamagnetic; however, they have to have a larger volume than the individual superparamagnetic nanoparticles. That can be achieved by controlled agglomeration of the superparamagnetic nanoparticles into clusters of appropriate size. Different procedures enabling the controlled agglomeration (self-assembly) of the nanoparticles

Basic conditions for the preparation of column-like Co-ferrite structures with the directed assembly of nanoparticles in a magnetic field were determined.

in their suspensions were systematically studied. The agglomeration was enabled by applying attractive electrostatic forces between the nanoparticles displaying an opposite surface charge, chemical reactions between the molecules on the nanoparticles' surfaces, or changes in the hydrofilicity of the medium.

We continued our research on the synthesis of nanocomposite particles used for the decomposition of or-

ganic pollutants in water. The nanocomposite particles are composed of photocatalytic anatase (TiO<sub>2</sub>) nanoparticles coated onto agglomerates of superparamagnetic maghemite (Fe<sub>2</sub>O<sub>2</sub>) 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 in cooperation with, and financing from, the company Cinkarne Celje, which was mainly devoted to the development of procedures for the industrial production of the materials, the basic research was also conducted. This research was manly oriented in mechanisms enabling an increase in the photocatalytic activity of the materials. This photocatalytic activity can be improved by the optimization of the nanocomposite structure, which significantly increases the effective specific surface area of the photocatalyst, or with optimization of the electronic properties of the anatase nanoparticles using the incorporation of dopants into their structure. In doping, the problem is mainly related to the incorporation of the appropriate concentration of a dopant in the anatase structure already during the nanoparticles' synthesis, which Figure 3: Columnar magnetic structures obtained by the magnetically usually takes place in an aqueous medium at relatively low temperatures. Chemical reactions enabling the incorporation of an acceptor dopant Fe<sup>3+</sup>

100 µm SUBSTRATE

directed assembly of Co ferrite nanoparticles

and a donor dopant W<sup>6+</sup> into the anatase structure of the nanoparticles during their synthesis using co-precipitation from aqueous solutions or hydrothermal method were studied.

Nanocomposite particles were also studied in the frame of the international applied project FOMS. The aim of this project is to develop a material and technology for the production of magneto-optic fibres suitable for magnetostrictive sensors. K8 was involved in a study of the synthesis of CoFe<sub>2</sub>O<sub>4</sub> nanoparticles and CoFe<sub>2</sub>O<sub>4</sub>/SiO<sub>2</sub> nanocomposites. The nanoparticles proved not to be suitable because of their low mass. Consequently, a too small fraction of particles was deposited on a glass substrate during the preform formation. As an alternative solution we prepared composite particles that consisted of CoFe<sub>2</sub>O<sub>4</sub> nanoparticles coated with SiO<sub>2</sub>. The fraction of up to 10 micron-sized composite particles, obtained after milling and size separation, was successfully incorporated into a preform, from which magneto-optic fibres were produced by our project partner Optacore. The presence of  $COFe_{a}O_{4}$  nanoparticles in those fibres was confirmed at K8 using transmission electron microscopy and from the magnetic measurements.

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 the 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. 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 perpen-

dicular to the electrode (i.e., the substrate). The direction of the hydrodynamic flow changes in the vicinity of an electrode and, consequently, the plates reorient in parallel to the electrode. New, incoming plates preferentially fill the empty space on the electrode due to electro-osmosis and the new layer is formed after the first one. We found that the orientation of the particles in the deposits depends on the particle size and the shape anisotropy, stability

Composite particles of Co ferrite in silica, suitable for incorporation in magnetooptic fibres, were prepared.

and conductivity of a suspension, the electrophoretic mobility, applied electric field and the EPD time. Since specific parameters depend on each other it is rather challenging to predict their common influence on the deposit's orientation. In general, the orientation degree of the deposits increases with the increasing shape anisotropy and

A mechanism for the orientation of Ba hexaferrite nanoparticles during the EPD was proposed on the basis of the mutual effects of electric and hydrodynamic forces. suspension stability, and with the decreasing electric field. Based on these findings, the EPD was optimized by increasing the operating voltage in steps. Using such a procedure we can prepare  $BaFe_{12}O_{19}$  deposits with thicknesses up to 25 microns and films with around 90% magnetic orientation after sintering at 950-1150°C. These films are suitable for application in the remanent state (i.e., without an applied magnetic field). In parallel, we continued with our studies on the deposition of  $BaFe_{12}O_{19}$  nanopar-

ticles in a magnetic field. This method results in films with a similar orientation degree

of the films as the EPD, but it has an advantage over the EPD: there is no need for a conductive substrate, which is not suitable for high-frequency applications. Our last experiments showed that the homogeneity of the deposits can be increased significantly by the application of a very weak magnetic field instead of a strong one.  $BaFe_{12}O_{19}$  nanoparticles are ferrimagnetic and are attracted to a weak magnet. A magnetic field of 0.02 T was strong enough for the preparation of films with around 90% of magnetic orientation after sintering at 1150°C.

The above-described studies served us as a basis for the realisation of an international applicative project FERFIT under the coordination of K8. The project has been conducted for two years, already. The aim of the project is to



Figure 4: Ba hexaferrite nanoplates for the preparation of oriented films

develop methods for the preparation of magnetically oriented films based on BaFe<sub>12</sub>O<sub>19</sub>. Such films can be applied as self-biased nonreciprocal devices. We aim at applications at 30-40 GHz. Therefore, a partial substitution of Fe<sup>3+</sup> in the BaFe<sub>12</sub>O<sub>19</sub> is required. K8 studied the substitution of In<sup>3+</sup> or Cr<sup>3+</sup> (BaM<sub>x</sub>Fe<sub>12.</sub>  $_{N_{19}}$ , M = In ali Cr) using hydrothermal synthesis. This year we focused on the influence of a substituent on the particle size. We noticed that a small In<sup>3+</sup> substitution for Fe<sup>3+</sup> (x = 0.2-0.3) significantly affects the particle size, which is more homogeneous than in the case of pure BaFe<sub>12</sub>O<sub>19</sub>. In<sup>3+</sup>-substituted particles are, on average larger, when synthesized at low temperature (160°C) than those of BaFe<sub>12</sub>O<sub>19</sub>, while they are smaller, on average, when synthesized at higher temperatures (200-240°C). Furthermore, the same effect was also observed for the Sc<sup>3+</sup>, while Cr<sup>3+</sup> showed no significant effect on the particle growth in comparison to the pure BaFe<sub>12</sub>O<sub>19</sub>. In<sup>3+</sup> and Sc<sup>3+</sup> are both larger than Fe<sup>3+</sup>, while Cr<sup>3+</sup> is of a more similar size to Fe<sup>3+</sup>. At the same time Cr<sup>3+</sup> does not precipitate completely under the synthesis conditions. We suppose

that at least one of these two differences causes different particle growth under hydrothermal conditions. Stable suspensions were prepared from the synthesized particles in 1-butanol with a surfactant dodecylbenzenesulphonic acid and were deposited in a magnetic field. The films with the highest magnetic orientation degree (around 95%) were obtained from the BaCrFe<sub>11</sub>O<sub>19</sub> of highly inhomogeneous size (diameter of 10-100 nm and thickness of 3-8 nm) after sintering at 1150°C.

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  $SrNb_2O_6$  and  $BaTiO_3-Na_{0.5}Bi_{0.5}TiO_3$ . In the latter 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

- Kralj, Slavko, Drofenik, Mihael, Makovec, Darko. Controlled surface functionalization of silica-coated magnetic nanoparticles with terminal amino and carboxyl groups. *J. nanopart. res.*, 2011, vol. 13, issue 7, str. 2829-2841, doi: 10.1007/s11051-010-0171-4.
- Primc, Darinka, Drofenik, Mihael, Makovec, Darko. Low-temperature hydrothermal synthesis of ultrafine strontium hexaferrite nanoparticles. *European Journal of Inorganic Chemistry*, 2011, vol. 2011, no. 25, str. 3802-3809, doi: 10.1002/ejic.201100326.
- 3. Lisjak, Darja, Ovtar, Simona. Directed assembly of BaFe[sub](12)O[sub](19) particles and the formation of magnetically oriented films. Langmuir, 2011, vol. 27, issue 23, str. 14014-14024, doi: 10.1021/la2032863.

#### Patent granted

 Photocatalytic TiO<sub>2</sub> coatings on superparamagnetic carriers and procedure of their production Darko Makovec, Dejan Verhovšek, Marjan Sajko SI23210 (A), Urad RS za intelektualno lastnino, 31.5.2011.

#### Annual Report 2011

# Awards and appointments

- 1. Marin Berovič, Darko Makovec: 2nd award for innovation at 4th International Conference of Technology Transfer, Ljubljana, IJS, Magnetisation of wine yeast and separation in production of sparkling wine.
- 2. Darko Makovec, Zoran Samardžija: Best poster contribution EMAS 2011 (European Microbeam Analysis Society, Angers), France, for poster "EPMA-WDS quantitative compositional analysis of barium titanate ceramics doped with cerium".
- 3. Slavko Kralj: 3. award for innovation UL; Dean's award for best innovation at UL, Ljubljana, proposer Ljubljana University Incubator (LUI) and University of Ljubljana (UL), Multifunctional nanoparticles for biomedical applications.

# INTERNATIONAL PROJECTS

- Composites with Novel Functional and Structural Properties by Nanoscale Materials (Nano Composite Materials NCM) COST MP0701 EC; COST Office, Brussels, Belgium Prof. Darko Makovec
- Ferrite Thick Films for Integrated Circuits FERFIT MNT-ERA-NET II
- Asst. Prof. Darja Lisjak Fiber Optics Magnetostrictive Sensor 3. FOMS MNT-ERA-NET, MANUNET 3
- Techno Gr srl, Piedmont, Italy Asst. Prof. Daria Lisiak
- Room-Temperature Multiferroics Based on Y-type HexaferritesBI-BG/09-10-004 4. BI-BG/11-12-004
- Dr. Svetoslav Mihaylov Kolev, Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria Asst. Prof. Darja Lisjak
- 5 Magnetic Nanoparticles for Hyperthermia Application BI-HU/10-11-002 Dr. Anna Sztaniszlav, TKI-FERRIT Development and Manufacturing Ltd., Budapest, Hungary
  - Prof. Darko Makovec

# R & D GRANTS AND CONTRACTS

- 1. Patterns, Structural Self-assemly and Multiferroic States in Mixtures of Nanoparticles and Liquid Crystals Prof. Samo Kralj
- 2. Development of photocatalytic superparamagnetic nanocomposites for application in diminishing emissions of harmful pollutants into an environment Prof. Darko Makovec

# **RESEARCH PROGRAM**

1 Advanced inorganic magnetic and semiconducting materials Prof. Mihael Drofenik

# NEW CONTRACTS

- Development of a procedure for preparation of superparamagnetic photocatalytic 1 nanocomposite particles. Cinkarna Celie d. d.
- Prof Darko Makovec
- Deformulation and development of iron-oxide nanoparticles for pharmaceutical 2 applications. Lek d. d.
- Prof. Darko Makovec
- Optimization of iron oxide nanoparticles synthesis analytical and expert support 3. Lek d d

#### Prof. Darko Makovec

# **MENTORING**

## Ph. D. Thesis

1. Miloš Beković, Development of measurement procedures for determining the magnetic losses of magnetic fluids (mentor Anton Hamler; co-mentor Mihael Drofenik).

# VISITORS FROM ABROAD

- 1. Mario Sartori, METEC, Torino, Italy, 2-7 Oct 11
- Massimo Pasquale, INRIM, Torino, Italiy, 2-7 Oct 11 2.
- 3. Herve Guillon, Kemstream, Montpellier, France, 2-7 Oct 11
- Denis Đonlagić, FERI UNI-MB, Maribor, Slovenia, 2-7 Oct 11 4.
- 5. Stane Čampelj, Miha Kveder - OptaCore, Ljubljana, Slovenia, 2-7 Oct 11

# STAFF

#### Researchers

- 1. Prof. Mihael Drofenik\*
- Asst. Prof. Darja Lisjak
- 3. Prof. Darko Makovec, Head
- 4. Dr. Igor Zajo

## Postdoctorial associates

5. Dr. Sašo Gyergyek Asst. Prof. Matjaž Kristl\*

## Postgraduates

#### Peter Dušak, B. Sc.

8. Petra Jenuš, B. Sc.

9. Slavko Kralj, B. Sc.

- 10. Simona Ovtar, B. Sc. 11. Darinka Primc, B. Sc.
- 12. Klementina Pušnik, B. Sc.
- 13. Aljaž Selišnik\*\*

Technical and administrative staff

14. Bernarda Anželak, B. Sc.

Note:

\* part-time JSI member \*\* postgraduate financed by industry

# BIBLIOGRAPHY

## **ORIGINAL ARTICLES**

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- Kirsten Bobzin, G. Bobelli, Markus Bruehl, Arto Hujanen, Pertti Lintunen, Darja Lisjak, Sašo Gyergyek, Luca Lusvarghi, "Characterisation of plasma-sprayed SrFe<sub>12</sub>O<sub>19</sub> coatings for electromagnetic wave absorption", *J. Eur. Ceram. Soc.*, vol. 31, issue 8, pp. 1439-1449, 2011.
- 3. Boštjan Denac, Matjaž Kristl, Mihael Drofenik, "Thermal behavior of nanocrystalline cadmium selenides and tellurides", *Chalcogenide Lett.*, vol. 8, no. 7, pp. 427-434, Jul. 2011.
- 4. Brina Dojer, Andrej Pevec, Marko Jagodič, Matjaž Kristl, Mihael Drofenik, "Three new cobalt(II) carboxylates with 2-, 3- and 4aminopyridine: syntheses, structures and magnetic properties", *Inorg. Chim. Acta*, Available online 31 October 2011.
- Mihael Drofenik, Irena Ban, Darko Makovec, Andrej Žnidaršič, Zvonko Jagličić, Darko Hanžel, Darja Lisjak, "The hydrothermal synthesis of super-paramagnetic barium hexaferrite particles: review", *Mater. chem. phys.*, vol. 127, iss. 3, pp. 415-419, 2011.
- 6. Mihael Drofenik, Gregor Ferk, Matjaž Kristl, Darko Makovec, "Synthesis and characterization of maghemite nanosheets", *Mater. lett.*, vol. 65, no. 3, pp. 439-441, 2011.
- Sašo Gyergyek, Darko Makovec, Mihael Drofenik, "Colloidal stability of oleic and ricinoleic acid coated magnetic nanoparticlesin organic solvents", *J. colloid interface sci.*, vol. 354, issue 2, pp. 498-505, 2011.
- 8. Svetoslav Kolev, Darja Lisjak, Mihael Drofenik, "Preparation and characterisation of magnetically ordered columnar structures of barium ferrite particles", *J. exp. nanosci. (Print)*, vol. 6, no. 4, pp. 362-373, 2011.
- 9. Slavko Kralj, Mihael Drofenik, Darko Makovec, "Controlled surface functionalization of silica-coated magnetic nanoparticles with terminal amino and carboxyl groups", *J. nanopart. res.*, vol. 13, issue 7, pp. 2829-2841, 2011.
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- Darja Lisjak, Marion Bégard, Markus Bruehl, Kirsten Bobzin, Arto Hujanen, Pertti Lintunen, Giovanni Bolelli, Luca Lusvarghi, Simona Ovtar, Mihael Drofenik, "Hexaferrite/polyester composite coatings for electromagnetic-wave absorbers", *J. therm. spray technol.*, vol. 20, no. 3, pp. 638-646, 2011.
- 12. Darja Lisjak, Pertti Lintunen, Arto Hujanen, Tommi Varis, Giovanni Bolelli, Luca Lusvarghi, Marko Jagodič, Mihael Drofenik, "Hexaferrite/polyethylene composite coatings prepared with flame spraying", *Mater. lett.*, vol. 65, no. 3, pp. 534-536, 2011.
- 13. Darja Lisjak, Simona Ovtar, "Directed assembly of BaFe<sub>12</sub>O<sub>19</sub> particles and the formation of magnetically oriented films", *Langmuir*, vol. 27, issue 23, pp. 14014-14024, 2011.
- 14. Darja Lisjak, Simona Ovtar, Mihael Drofenik, "The stability of BaFe<sub>12</sub>O<sub>19</sub> nanoparticles in polar solvents", *J. Mater. Sci.*, vol. 46, no. 9, pp. 2851-2859, 2011.
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- Alenka Mertelj, Andraž Rešetič, Sašo Gyergyek, Darko Makovec, Martin Čopič, "Anisotropic microrheological properties of chain-forming magnetic fluids", Soft matter, vol. 7, issue 1, pp. 118-124, 2011.
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Conference YUCOMAT 2010, Herceg Novi, Montenegro, *Acta Phys. Pol.*, *A*, vol. 120, no. 2, pp. 316-321, 2011.

- 20. D. Milivojević, Branka Babić-Stojić, Vukoman Jokanović, Zvonko Jagličić, Darko Makovec, "Magnetic properties of Mn-oxide nanoparticles dispersed in an amorphous SiO2 matrix", *J. magn. magn. mater.*, vol. 323, no. 6, pp. 805-812, 2011.
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- 22. Jana Padežnik Gomilšek, Alojz Kodre, Iztok Arčon, Simone De Panfilis, Darko Makovec, "Atomic absorption background of Ba in EXAFS analysis of BaFe12019 nanoparticles", *J. synchrotron radiat.*, vol. 18, issue 4, pp. 557-563, 2011.
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- 24. Brigita Rožič, Marko Jagodič, Sašo Gyergyek, Mihael Drofenik, Samo Kralj, George Cordoyiannis, Zdravko Kutnjak, "Multiferroic behaviour in mixtures of the ferroelectric liquid crystal and magnetic nanoparticles", In: Proceedings of the 23rd International Liquid Crystal Conference (ILCC 2010), *Mol. Cryst. Liq. Cryst.*, vol. 545, no. 1, pp. 99-104, 2011.
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## PUBLISHED CONFERENCE PAPERS

#### **Regular** papers

- 1. Irena Ban, Matjaž Kristl, Mihael Drofenik, "A sonochemical method for the preparation of CdTe nanoparticles for photovoltaic cells", In: *Book of abstracts, Proceedings book,* Slovenian-Italian Conference on Materials and Technologies for Sustainable Growth, Ajdovščina, 4-6 May 2011, Matjaž Valant, ed., Sandra Gardonio, ed., Elsa Fabbretti, ed., Urša Pirnat, ed., Nova Gorica, University, 2011, pp. 1-[8].
- Marin Berovič, Darko Makovec, Suzana Bošković, Matjaž Berlot, "New method for fast separation of magnetized yeast Saccharomyces cerevisiae from sparkling wine: [lecture]", In: *The wine construction*, XXXIV World Congress of Vine and Wine, 20-27th June 2011, Porto, Portugal, [Lisboa, Ministry for Agriculture, Rural Development and Fishing], 2011, pp. [1-5].
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- 4. Gregor Ferk, Irena Ban, Janja Stergar, Darko Makovec, Mihael Drofenik, "Priprava magnetnih Mg<sub>1+x</sub>Fe<sub>2-2x</sub>Ti<sub>x</sub>O<sub>4</sub> nanoprahov s soobarjanjem za namene hipertermije", In: *Slovenski kemijski dnevi 2011, Portorož, 14-16 september 2011,* Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2011, 6 pp.
- Petra Jenuš, Darja Lisjak, Darko Makovec, Mihael Drofenik, "Priprava nanokompozitov (COFe<sub>2</sub>O<sub>4</sub>/BaTiO<sub>3</sub>) po vplivom zunanjih polj", In: *Slovenski kemijski dnevi 2011, Portorož, 14-16 september 2011*, Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2011, pp. 1-8.
- 6. Petra Jenuš, Darja Lisjak, Darko Makovec, Mihael Drofenik, "Priprava stopličastih struktur CoFe<sub>2</sub>O<sub>4</sub> pod vplivom magnetnega polja", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 168-174.
- 7. Matjaž Kristl, Irena Ban, Mihael Drofenik, "Mechanical alloying as a facile route to the synthesis of semiconducting chalcogenides", In: *Book of abstracts, Proceedings book*, Slovenian-Italian Conference on Materials and Technologies for Sustainable Growth, Ajdovščina, 4-6

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- 10. Darinka Primc, Mihael Drofenik, Darja Lisjak, Darko Makovec, "Magnetne lastnosti nanodelcev Ba heksaferita (BaFe<sub>12</sub>O<sub>19</sub> sintetiziranih s hidrotermalno sintezo", In: Zbornik prispevkov, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 190-195.
- 11. Brigita Rožič, Zdravko Kutnjak, George Cordoyiannis, Boštjan Zalar, Slobodan Žumer, Simon Krause, Heino Finkelmann, Barbara Malič, Alja Kupec, Janez Holc, Marija Kosec, Raša Pirc, Robert Blinc, Marko Jagodič, Sašo Gyergyek, Mihael Drofenik, Samo Kralj, Gojmir Lahajnar, Zvonko Jagličić, "Liquid crystal elastomers, electrocalorics, and new soft magnetoelectrics: materials for advanced technologies", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana,

Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 199-205.

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#### **TEXTBOOKS AND LECTURE NOTES**

1. Darja Lisjak, *Physical and chemical properties of nanoparticles: electrooptical and chemical properties*, Ljubljana, Jožef Stefan International Postgraduate School, 2011.

### B. Sc. Thesis

1. Slavko Kralj, *Academic entrepreneurship: business plan for a nanotech company:* undergraduate thesis, Ljubljana, [S. Kralj], 2011.

#### PATENT

1. Darko Makovec, Dejan Verhovšek, Marjan Sajko, *Photocatalytic TiO2* coatings on superparamagnetic carriers and procedure of their production, SI23210 (A), Urad RS za intelektualno lastnino, 31.5.2011.

# DEPARTMENT FOR ADVANCED MATERIALS

K-9

The primary activities of the department are the development of new materials and the new processes needed for the preparation of such materials in the form of nanostructures and nanocomposites. The main objective of current projects is the synthesis of new, environmentally friendly materials with special electrical and optical properties, with the emphasis on tunable materials that exhibit a dependence of the electric polarization on external electric, mechanical or magnetic fields. A significant part of the research is devoted to the development of new ceramic dielectrics that can be used at microwave frequencies. A new field of the department's research is aimed at the synthesis of photocatalytically active and antibacterial nanocomposites for their wide area of potential applications: from domestic appliances to medicine.

#### Development of materials with special electrical properties

Thermoelectric materials have been extensively studied in the last decade, as a possible sustainable solution to the imminent energy problem. The studied materials have the ability to transform the generated heat directly into Head electrical energy and can therefore be used as a waste-heat collector, in, for example, exhaust systems or they can Prof. Danilo Suvorov directly transform the heat generated by chemical or nuclear reactions into electricity. Theoretically, it was predicted that the efficiency of such a device should reach a 100% efficiency of the Carnot cycle; however, only a moderate output was achieved so far. Our study has focused on oxide ceramic semiconductors that are seen as candidates for high-temperature applications, where conventional alloys fail. Among the known oxide thermoelectric, Na CoO, was reported to exhibit the highest efficiency among p-type thermoelectric oxides. There are, however, severe discrepancies in the reported values, which are not yet understood. Our aim was to prepare a phase-pure ceramic material with a well-defined microstructure, which has so far, based on published results, not yet been realized We employed several different synthesis techniques such as solid-state and sol-gel, to synthesize the Na<sub>x</sub>CoO<sub>2</sub> (0.55<x<0.85). We investigated the chemical properties, such as temperature stability and reactivity under different atmospheres,

and in different solvents. We found that Na CoO<sub>2</sub> is very sensitive to water molecules that cause a broadening of the unit cell and, consequently, if the water content is high enough, transform a solid pellet into a gel-like paste. By avoiding moisture in the next steps of the material processing, we have optimized the synthesis process, which gives reproducible results, at least in terms of the microstructure of such ceramics. In order to prevent contamination of the material with moisture we developed an appropriate protective paste, which covers the material well. We also developed a conductive paste to ensure good electrical contact with the measuring instrument, or enables the integration of an application-device. On the other hand, the unusually

high average oxidation state of Co is prone to changes at temperatures in the vicinity of 800°C. For the densification of the powder temperatures above 950°C, which is above the decomposition temperature in an air atmosphere, are required. Our findings indicate that high pressures of oxygen need to be employed during the processing of the Na COO<sub>2</sub> ceramics. The thus prepared material withstands temperatures up to 930°C in an air atmosphere and is therefore a potential candidate for a p-type thermo-element in high-temperature thermoelectric modules.

Another part of the research was focused on understanding the formation mechanism of ferroelectric K<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>2</sub> ceramics. Control of the solid-state synthesis parameters enabled us to prepare dense K<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>2</sub> ceramics with a minor part of secondary phases, which ensures that the measured electrical properties can be ascribed to the matrix phase. An analysis of the electrical properties revealed an improvement with the extension of the sintering time and, moreover, the peculiarities became sharper. For example, the frequency dispersion of the dielectric properties became smaller, the peaks become sharper and the squareness of the ferroelectric hysteresis increased. After a shorter sintering time the samples exhibit increased conductivity; this deteriorates their electrical properties. Such behavior was connected with the presence of a K<sub>2</sub>O-rich secondary phase, concentrated on the grain boundaries. This phase is in a melted state at the sintering temperature and reacts with humidity from the atmosphere. With a prolonged sintering time this phase volatizes and redistributes, which decreases its continuity within the ceramics. Consequently, the resistivity increases and the electrical properties improve for sintering times longer than 15 hours. A characterization of the electrical properties showed the superior properties of the as-prepared samples



For the applicability of oxide thermoelectric Na CoO, we have developed an appropriate protection paste, which covers well the material, and prevents the material's contamination with moisture. We have also developed a conductive paste to ensure good electrical contact with the measuring instrument, or enable the integration of an application device.

compared to the literature. The relative permittivity and losses at room temperature and 1 MHz are higher than 500 and smaller than 7%, respectively, whereas the permittivity at the maximum is higher than 5400. The remanent polarization and coercive field were  $30 \,\mu\text{C/cm}^2$  and  $63 \,\text{kV/cm}$ , respectively, which indicates strong ferroelectricity and the "hard" nature of the  $K_{0.5}Bi_{0.5}TiO_3$  ceramics. Field cooling at 50 kV/cm was performed from 250°C to below 100°C. Under these conditions the piezoelectric coefficient ( $d_{33}$ ) was as high as 115 pC/N, which is higher than in related  $Na_{0.5}Bi_{0.5}TiO_3$ . With a potassium non-stoichiometry the dielectric and ferroelectric properties rapidly degrade. However, the piezoelectric properties remain relatively high, with  $d_{33}$  values between 75 and 90 pC/N, in samples with -4% to +2% of potassium compared to the stoichiometric  $K_{0.5}Bi_{0.5}TiO_3$ .

In the scope of an applied project with EPCOS OHG, Deutschlandsberg, Austria, ferroelectric ceramics from the Pb(Zn<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-BaTiO<sub>3</sub>-PbTiO<sub>3</sub> (PZN-BT-PT) and (Pb<sub>1x</sub>Sr<sub>x</sub>)(Zr<sub>0.538</sub>Ti<sub>0.438</sub>Nb<sub>0.024</sub>)O<sub>3</sub> (PSZTN) perovskite systems were investigated as potential materials for applications in power electronics. For both systems the variations of the ferroelectric (T<sub>c</sub>,  $\varepsilon_{max}$ ) and structural characteristics were examined as a function of the composition. In the PZN-BT-PT system compositional changes enabled a variation of the Curie temperature (T<sub>c</sub>) from 100 to 200°C and a dielectric constant maximum ( $\varepsilon_{max}$ ) from 8000-11000. The PSZTN compositions exhibit T<sub>c</sub>=150-250°C and  $\varepsilon_{max}$ =8000-12000. The investigations of the field dependence of the dielectric constant revealed that electric fields of 70-100 kV/cm lowered the e values by 80-95%.

#### **Development of microwave dielectrics**

In the investigations of the microwave dielectric materials we have studied the influence of the sintering temperature and different atmospheres on the densification, decomposition of the matrix, and the homogeneity of the components with respect to their dielectric properties in the microwave-frequency region.

We have observed that during the preparation of  $Ag(Nb_{1x}Ta_x)O_3$  ceramics the oxidation and reduction processes of Ag cause problems related to the matrix decomposition and densification. At low sintering temperatures (1040–1080 ° C) the secondary phases related to the heterogeneous distribution of the Nb and Ta appears in addition to the matrix phase. When the sintering temperatures are between 1120 and 1200 °C the homogeneity of the components are improved due to the higher diffusion rates, but on the other hand  $Ag(Nb_{0.5}Ta_{0.5})O_3$  partially decomposed into  $Ag_2(Nb,Ta)_4O_{11}$ ,  $Ag_8(Nb_{0.5}Ta_{0.5})_{26}O_{69}$  and Ag. Consequently, sintering in air did not result in a single-phase  $Ag(Nb_{0.5}Ta_{0.5})O_3$  ceramic. We observed that sintering in pure oxygen under increased pressure retarded the decomposition process according to Le Chatelier 's principle and as a result we were able to synthesize predominantly single-phase ceramics with a high density. Nevertheless, a sample sintered at 1080 °C in air exhibited optimal dielectric properties; i.e.,  $\varepsilon \approx 440$ ,  $Q \times f \approx 622$  GHz, and  $\tau_f \approx -16$  ppm/K. We also described how the Nb and Ta distributions in the  $Ag(Nb_{0.5}Ta_{0.5})O_3$  material influence the temperature coefficient of the resonant frequency.

In the investigation of MgO-B<sub>2</sub>O<sub>3</sub>–SiO<sub>2</sub> (MBS) glass ceramic we have studied the effect of TiO<sub>2</sub> as nucleating agent on the nucleation and crystallization processes using several kinetic methods based on non-isothermal DSC measurements. According to the XRD examination after the DSC measurements the Mg<sub>2</sub>B<sub>2</sub>O<sub>5</sub> phase is the main phase in samples with and without a nucleating agent. Selected-area electron diffraction (SAED) confirmed the Mg<sub>2</sub>B<sub>2</sub>O<sub>5</sub> structure of the newly formed phase. The crystallization peak temperature is shifted to lower temperatures and the DSC peak became narrower and more intense with the increase of TiO<sub>2</sub> content. Small additions of TiO<sub>2</sub> (<3 wt. %) were found to have no significant effect on the DSC curve, while the higher concentrations of TiO<sub>2</sub> (>3



Figure 1: Together with Nanocenter CONIN we have obtained a probe station for the electrical characterization of ceramic thin films (a). In the low-frequency range the electrical measurements were performed by the method of parallel capacitors, where a thin layer is sandwiched between two electrodes (b), while in the microwave range the used method is the planar capacitor configuration, where the electrode is applied only on one side of the thin film (c).

wt. %) resulted in the substantial lowering of the crystallization peak (Tp) temperature, which is caused by a high nuclei concentration. The influence of  $\text{TiO}_2$  on the growth mechanism was followed by the variation of the Avrami exponent (n), determined by the Ozawa relation, and its relation to the morphology index (m'). The variation of n with  $\text{TiO}_2$  content thus reflected the changes in the nucleation rate and the growth-controlling mechanism. The increase of n from 1.5 to 2.5 at 3 wt. % TiO<sub>2</sub> indicated the change from zero to a constant nucleation rate. With a further increase of TiO<sub>2</sub>, n changed to 4 and the crystal growth rate became interface controlled with a constant nucleation rate.

The miniaturization of electronic components favors the replacement of bulk ceramic components with thin-film-based components. One of the methods for the preparation of thin films is the sol-gel method. As part of our thin-film investigation we have studied the influence of heat-treatment conditions (pyrolysis and annealing) on the microstructural development of the 70 mol%  $Na_{0.5}Bi_{0.5}TiO_3 - 30$  mol%  $NaTaO_3$  thin films. We have observed that by using a one-step pyrolysis and annealing at different temperatures, the obtained thin films show a markedly different microstructure. In the case of using two-step pyrolysis, we have obtained similar microstructures of thin films, regardless at which temperatures we annealed. Such a microstructure displays a columnar grain growth. We have also fabricated multilayer  $SrTiO_3/NaO_5Bi_{0.5}TiO_3$  thin films. The preparation of multilayers by employing a dielectric layer between the ferroelectric film and the electrodes enabled us to prepare ferroelectric thin films that exhibit lower values of leakage current as compared to pure  $SrTiO_3$  or  $Na_{0.5}Bi_{0.5}TiO_3$  films. We have observed that such multilayered structures offer the possibility to improve the electrical characteristics required to achieve applicability and long-lasting reliability of the prepared ferroelectric layers.

The microwave dielectric (MW) properties of ceramic thin films can be determined with the split-post dielectric resonator methods as well as with a planar capacitor measurement configuration, where the interdigital electrodes are a pattern on the same side of the thin film. We were particularly focused on the study of MW dielectric properties of the planar capacitor configuration, which provides MW data over the whole microwave-frequency region. The measuring capacitance must be within the range of  $0.03 \text{ pF} \le C \le 3 \text{ pF}$  and can be varied by the design of interdigital electrode structures (Fig. 1), which influences the accuracy of the measuring data. Therefore, the combination of the analytical and numerical modeling for co-planar interdigital electrode structures was used to characterize the dielectric properties of ceramic thin films. The co-planar interdigital electrode structures were prepared using E-beam lithography.

#### Research of nanostructured materials and nanocomposites

a.) Nanoparticles and nanopowders

The material synthesis approach turns out to be the key parameter in obtaining improved properties of the ceramics. The research of nanostructured materials has been focused on the synthesis of  $BaTiO_3$  and  $CoFe_2O_4$  nanoparticles prepared by hydrothermal or solvothermal synthesis.

The BaTiO<sub>3</sub> nano-particles with various morphologies were prepared under different hydrothermal and solvothermal synthesis conditions. We studied the influence of solvent, temperature, concentration and type of the precursors on the shape, crystal structure and size of the synthesized particles. BaTiO<sub>3</sub> particles were formed in alkaline solutions of barium precursors from TiO<sub>2</sub> or sodium titanate nanostructures at 100-230°C. BaTiO<sub>3</sub> particles in the shape of spheres, stars, rods and squares were obtained using different synthesis conditions (fig. 2).

We prepared a ceramic material with artificially created nanostructures. The ordered nanostructures, which consisted of nano-dots or nano-circles of  $\beta$ -Bi<sub>2</sub>O<sub>3</sub>, were manufactured using electron lithography and the sol-gel method.

Cobalt ferrite nanoparticles were prepared via the precipitation-hydrothermal method. The influences of pH and temperature on the structural and magnetic properties were investigated. We observed that with the pH increases the crystallinity and the average particle size increase. The crystallinity of the samples also increased with increased temperature. However, only small changes in the particle size were observed. The results of the magnetic measurement revealed that the increase of temperature and pH causes an increase of the saturation magnetization, remanent magnetization and coercivity of the cobalt ferrite nanoparticles.

In the field of colloidal and nanomaterials, nanostructured spherical particles of  $MnCO_3$ , with the size of 2 µm were prepared by using a biomimetic synthesis method. Further thermal treatment of these particles at different temperatures and in different atmospheres resulted in the formation of nanostructured particles of MnO,  $Mn_2O_3$  in  $Mn_3O_4$ . In a study of the CaCO<sub>3</sub> particles' growth in an aqueous medium, we identified a range of complex and nanostructured particles with different crystal structure. Samples were prepared from different precursors with or without the presence of different enzymes that act as templates (base) in the growth of particles and affect the crystal structure and morphology of the generated particles.



Figure 2: The morphology of the  $BaTiO_3$  particles formed from sodium titanate belts in alkaline water solution (a) and in water/ethanol (75/25) alkaline solution (b) at 100°C.

#### b.) Nanocomposites

The fabrication of nanostructured thin films consisting of hybrid materials based on semiconducting titania and titanate nanostructures have recently been the subject of intense research arising from their enhanced semiconducting properties that have widespread potential for application in photocatalysis, catalysis, photovoltaic's and gas sensing.

The nanocomposites based on  $\text{TiO}_2/\text{Pt}$  were prepared by the sol-precipitation method followed by thermal treatment in a reducing atmosphere at 400°C for 3h. These so prepared  $\text{TiO}_2/\text{Pt}$  nano-composites were a biphasic  $\text{TiO}_2$ , consisting of anatase (average particle size 14 nm) and rutile (average particle size 15 nm), which were attached with Pt particles (3-15 nm). The measured specific surface area of such nano-composites was 62 m<sup>2</sup>/g. The photocatalytic activities of the  $\text{TiO}_2/\text{Pt}$  nano-composites, determined under ultraviolet (UV) irradiation in gaseous



Figure 3: Ordered nanostructures consisted of a) nano-dots or b) nanocircles of  $\beta$ -Bi<sub>2</sub>O<sub>3</sub> prepared by using electron lithography and the sol-gel method.

media (photocatalytic oxidation of isopropanol), exceeded the photocatalytic efficiency of the bare  $\text{TiO}_2$  nano-powders. The enhancement of the UV photocatalytic activity with the  $\text{TiO}_2/\text{Pt}$  when compared to the bare  $\text{TiO}_2$  was also observed in aqueous media for the photocatalytic discoloration of an azo-dye solution of methylene blue.

In the field of photo-catalytic processes an effective approach to expand the photoactive range and enhance the activity of titanate-based 1D nanostructures has been achieved by coupling the wide-semiconducting titanate nanobelts (Ti-NBs) with the metallic (Cu) or narrow-band-gap (CuO) semiconducting nanoparticles. For the CuO/Ti-NBs and Cu/Ti-NBs film fabrication the weak-polyelectrolyte multilayer (PEM) coated Ti-NBs were subsequently utilized as a nanoreactor for the *in-situ* synthesis of metallic Cu nanoparticles. The as-synthesized single-crystalline fcc Cu nanoparticles are spherical and uniformly distributed within the PEM on the surface of the Ti-NBs. The as-formed Cu-loaded PEM/Ti-NBs precursor structures were then utilized for the fabrication of 10 and 20 bilayered film assemblies with the layer-by-layer self-assembly methodology. The cross-sectional FE-SEM images of 10 and 20 layered Ti-NBs films revealed that multilayered films formed by the layer-by-layer assembly yield the orientation of Ti-NBs in the film, which is not parallel with the substrate. This induces nanoscale porosity and yields a high specific area of the as-formed nanostructured films, making as-formed multilayered Ti-NB thin films an ideal potential photocatalytic structure for the degradation of organic contaminants.

The ability to manipulate the internal structure of materials at nanometer-length scales and control the dimensions of nanostructures is in the forefront of current research for multi-functional materials. Therefore, part of our research was focused on the preparation of ceramic materials with artificially created nanostructures. By using electron lithography and the sol-gel method we had ordered nanostructures consisting of nano-dots or nano-circles of  $\beta$ -Bi<sub>2</sub>O<sub>3</sub> (Fig. 3).

## Some outstanding publications in the past year

- 1. Marija Vukomanović, Ines Bračko, Ida Poljanšek, Dragan Uskoković, Srečo D. Škapin, Danilo Suvorov, "The growth of silver nanoparticles and their combination with hydroxyapatite to form composites via a sonochemical approach", *Cryst. growth des.*, vol. 11, issue 9, pp. 3802-3812, 2011
- Mojca Otoničar, Srečo D. Škapin, Boštjan Jančar, "TEM analyses of the local crystal and domain structures in (Na<sub>(1-x)</sub>K<sub>x</sub>)<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> perovskite ceramics", *IEEE trans. ultrason. ferroelectr. freq. control*, vol. 58, no. 9, pp. 1928-1938, 2011
- Matjaž Spreitzer, Danilo Suvorov, "Electrical characteristics of Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub>-Li<sub>0.45</sub>La<sub>0.52 0.03</sub>TiO<sub>3</sub> system", *J. Am. Ceram. Soc.*, vol. 94, issue 7, pp. 2104-2108, 2011
- 4. Marjeta Maček, Manca Logar, Bojan Budič, Danilo Suvorov, "Dielectric and microstructural study of the SrWO<sub>4</sub>, BaWO<sub>4</sub>, and CaWO<sub>4</sub> scheelite ceramics", *J. Am. Ceram. Soc.*, vol. 94, no. 8, pp. 2464-2472, 2011
- Ines Bračko, Boštjan Jančar, Manca Logar, Dejan Caglič, Danilo Suvorov, "Silver nanoparticles on titanate nanobelts via the self-assembly of weak polyelectrolytes: synthesis and photocatalytic properties", *Nanotechnology* (*Bristol*), vol. 22, issue 8, pp. 085705-1-085705-11, 2011

## Awards and appointments

- 1. Andreja Šestan: Award for contribution to the sustainable development of society for the year 2010, Ljubljana, The Slovene Human Resources and Scholarship Fund, Microstructure characteristics of materials based on Ni-GDC and GDC prepared by citrate-nitrate combustion synthesis.
- 2. Vojka Žunič: Award for contribution to the sustainable development of society for the year 2010, Ljubljana, The Slovene Human Resources and Scholarship Fund, Sol-gel synthesis of TiO2 nano-powders, which are photocatalytically active under visible light irradiation.
- Vojka Žunič: Award for the best poster, 10th Brazilian MRS Meeting, Gramado, Brazil, Brazilian Materials Research Society, Photocatalytic activity of TiO2 nano-powders prepared via two different synthesis methods.

## Organization of conferences, congress and meetings

- 1. Brazilian Slovenian Workshop on synthesis methods of nanostructured materials, Araraquara, Brazil, 19–23 September 2011 (co-organizers)
- 2. Materials Science & Technology 2011 Conference and Exhibition, Columbus, USA, 16 20 October 2011 (co-organizers)
- 3. 19th Conference on Materials and Technologies, Portorož, 22–23 November 2011 (co-organizers)
- 4. Workshop on MATERA ERA-NET project "Novel inorganic inks for hybrid printed electronic demonstrators", Ljubljana, 21–22 November 2011

# INTERNATIONAL PROJECTS

- 1. Development of Wear Resistant Coatings based on Complex Metallic Alloys for Functional Applications AppliCMA 7. FP, 214407 EC; Andreas Merstallinger, Aerospace & Advanced Composites GmbH, Wiener Neustadt, Austria Asst. Prof. Srečo D. Škapin, Asst. Prof. Miha Čekada, Prof. Janez Dolinšek, Asst. Prof. Kristoffer Krnel Novel Inorganic Inks for Hybrid Printed Electronic Demonstrators INNOINKS MNT ERA NET University of Oulu (UOULU), Finland Prof. Danilo Suvorov Nanostructured Ferroelectric Films for Biosensor 3 NAFERBIO MNT ERA NET II Chalmers Tekniska Hogskola AB, Sweden Prof. Danilo Suvorov 4 Functional Nanostructured Ceramic Materials BI-AR/09-11-001 Prof. Noemí Elisabeth Walsõe de Reca, CINSO (Centro de Investigaciones en Sólidos), CITEFA-CONICET, Buenos Aires, Argentine Prof. Danilo Suvorov Thermoelectric Oxide Materials Agreement IJS/EPCOS, NBT Project Dr. Manfred Schweinzger, Hermann Gruenbichler, EPCOS OHG Ceramic Components Division, Deutschlandsberg, Austria Prof. Danilo Suvorov, Asst. Prof. Boštjan Jančar High K Dielectrics for Mobile Phone Base Stations 4502220319/302 Dr. Christian Hoffmann, Pavol Dudesek, EPCOS OHG Ceramic Components Division, Deutschlandsberg, Austria Prof. Danilo Suvorov High K Dielectrics for Mobile Phone Base Stations Agreement IJS/EPCOS, Microwave Ceramics Dr. Christian Hoffmann, Pavol Dudesek, EPCOS OHG Ceramic Components Division, Deutschlandsberg, Austria Prof. Danilo Suvorov, Asst. Prof. Boštjan Jančar 8. High Dielectric Constant Ferroelectric Material; Thermoelectric Oxide Materials Agreement IJS/EPCOS, NBT Dr. Guenter Engel, dr. Andrea Testino, EPCOS OHG Ceramic Components Division, Deutschlandsberg, Austria Prof. Danilo Suvorov, Dr. Marjeta Maček Kržmanc, Asst. Prof. Boštjan Jančar 9. High K Dielectrics for Mobile Phone Base Stations Agreement IJS/EPCOS, Microwave Ceramics Dr. Christian Hoffmann, Pavol Dudesek, EPCOS OHG Ceramic Components Division, Deutschlandsberg, Austria
- Prof. Danilo Suvorov, Asst. Prof. Boštjan Jančar
- The Synthesis of Dielectric Materials by Chemical Solution Deposition and Characterization of their Dielectric Properties BI-BR/11-13-002

# MENTORING

## Ph. D. Thesis

 Urban Došler, The synthesis and characterization of glass-ceramic based on ternary system MgO-B,O, SiO, (mentor Danilo Suvorov; co-mentor Marjeta Maček Kržmanc).

- Prof. José Arana Varela, Instituto de Quimica-UNESP, Araraquara, Brazil Prof. Danilo Suvorov
- 11. Ultra-low Dielectric Constant LTCC Material BI-CN/09-11-013
- Dr. Xing Hu, South China University of Technology, Guangzhou, China Asst. Prof. Srečo Davor Skapin
- Synthesis of Piezoelectric Thin Films and Magnetoelectic Composites by a Layer-by-layer Self Assembly BI-KR/09-11-001
  - Dr. Jae-Ho Jeon, Korea Institute of Materials Science, Changwon, Korea Prof. Danilo Suvorov
- Mixed Rare Earth Oxide Nanoparticles: Synthesis, Characterisation, Applications BI-SR/10-11-016
   Dr. Bratislav Antić, "Vinča" Institute of Nuclear Sciences, Beograd, Serbia Asst. Prof. Boštjan Jančar

# R & D GRANTS AND CONTRACTS

- 1. Nanoengineering of self-assembled materials Prof. Danilo Suvorov
- 2. Self-cleaning antibacterial fotocatalitic coatings in whitewear production Prof. Danilo Suvorov
- Functionalization of the surface of organic pigments for durable, efficient and colourstable paints Asst. Prof. Srečo Davor Škapin
- Physis and chemistry of porous aliminium for Al panels, capable of higly efficient energy absorbtion
- Prof. Danilo Suvorov5. New materials for power conversion: Oxide semiconductor thermoelectricsProf. Danilo Suvorov

# **RESEARCH PROGRAM**

1. Contemporary inorganic materials and nanotechnologies Prof. Danilo Suvorov

# NEW CONTRACTS

- 1. Development and characterisation of mineral wool fibres Knauf Insulation, d. o. o., Škofja Loka Prof. Danilo Suvorov
- Self-Cleaning antibacterial fotocatalitic coatings in whitewear productions Gorenje Household Appliances Prof. Danilo Suvorov
- New materials for energy conversion Gorenje Household Appliances Prof. Danilo Suvorov

# VISITORS FROM ABROAD

- 1. Ruben Zowada, B. Sc., Cascade Microtech Inc., München, Germany, 25 January 2011
- 2. Dr. Ivan Sondi, Rudjer Bošković Institute, Zagreb, Croatia, 24 February 2011
- Prof. Dragoljub Uskoković, Institute of Technical Sciences, SASA, Belgrade, Republic of Serbia, 16–17 March 2011
- Dr. Bratislav Antić, Vinča Institute of Nuclear Sciences, Belgrade, Republic of Serbia, 27 March to 1 April 2011
- Zoran Jovanović, B. Sc., Faculty of Physical Chemistry, University of Belgrade, Belgrade, Republic of Serbia, 1 April 2011
- 6. Gorazd Šebenik, B. Sc., Markus Mente, B. Sc., Knauf Insulation, Škofja Loka, 5 April 2011



- 7. Markus Mente, B. Sc., Knauf Insulation, Škofja Loka, 18 May 2011
- 8. Gorazd Šebenik, B. Sc., Knauf Insulation, Škofja Loka, 24 May 2011
- Dr. Smilja Marković, Institute of Technical Sciences, SASA, Belgrade, Republic of Serbia, 21 – 31 May 2011
- Prof. Ling Zhi Yuan, South China University of Technology, Gangzhou, China, 25 May to 3 June 2011
- 11. Dr. Hu Xing, South China University of Technology, Gangzhou, China, 25 May to 3 June 2011
- 12. Dr. Ivan Sondi, Rudjer Bošković Institute, Zagreb, Croatia, 16 June 2011
- Hermann Gruenbichler, B. Sc., Dr. Manfred Schweinzger, Yongli Wang, B. Sc., TDK EPCOS, Deutschlandsberg, Austria, 1 September 2011
- Dr. Jae Ho Jeon, Korea Institute of Material Science, Changwon, Korea, 10–13 September 2011
- Dr. Somnuk Sirisoonthorn, National Metal and Materials Technology Center, Pathumthani, Thailand, 13–14 October 2011
- Dr. Marija Vukomanović, Institute of Technical Sciences, SANU, Belgrade, Republic of Serbia, 23–24 October 2011
- Dr. Bratislav Antić, Vinča Institute of Nuclear Sciences, Belgrade, Republic of Serbia, 7–13 November 2011
- STAFF

#### Researchers

- 1. Asst. Prof. Boštjan Jančar
- 2. Dr. Marjeta Maček Kržmanc
- 3. Prof. Danilo Suvorov, Head
- 4. Asst. Prof. Srečo Davor Škapin
- Postdoctorial associates
- 5. Dr. Urban Došler
- 6. Dr. Jakob König
- 7. Dr. Uroš Kunaver\*
- 8. Dr. Špela Kunej
- 9. Dr. Manca Logar
- 10. Dr. Matjaž Spreitzer
- 11. Dr. Marko Udovič\*
- 12. Dr. Asja Veber
- Postgraduates

#### 13. Ines Bračko, B. Sc

# BIBLIOGRAPHY

## ORIGINAL ARTICLES

- 1. Gabriela Ambrožič, Srečo D. Škapin, Majda Žigon, Zorica Crnjak Orel, "The formation of zinc oxide nanoparticles from zinc acetylacetonate hydrate intert-butanol: a comparative mechanistic study with isomeric C4 alcohols as the media", *Mater. res. bull.*, vol. 46, issue 12, pp. 2497-2501, 2011.
- Gabriela Ambrožič, Srečo D. Škapin, Majda Žigon, Zorica Crnjak Orel, "Poly(zinc dimethacrylate) as a precursor in the low-temperature formation of ZnO nanoparticles", *J. colloid interface sci.*, vol. 360, issue 2, pp. 370-376, 2011.
- Ines Bračko, Boštjan Jančar, Manca Logar, Dejan Caglič, Danilo Suvorov, "Silver nanoparticles on titanate nanobelts via the selfassembly of weak polyelectrolytes: synthesis and photocatalytic properties", *Nanotechnology (Bristol)*, vol. 22, issue 8, pp. 085705-1-085705-11, 2011.
- 4. Marija Drev, Urša Opara Krašovec, Mateja Hočevar, Marko Berginc, Marjeta Maček, Marko Topič, "Pechini based titanium sol as a matrix in TiO<sub>2</sub> pastes for dye-sensitized solar cell application", *J. sol-gel sci. technol.*, vol. 59, no. 2, pp. 245-251, 2011.
- Andreja Gajović, Adrián M. T. Silva, Ricardo A. Sigundo, Sašo Šturm, Boštjan Jančar, Miran Čeh, "Tailoring the phase composition and morphology of Bi-doped goethite-hematite nanostructures and their catalytic activity in the degradation of an actual pesticide using a photo-Fenton-like process", *Appl. catal., B Environ.*, vol. 103, no. 3/4, pp. 351-361, 2011.
- 6. Dragana Jugović, Miodrag Mitrić, Maja Kuzmanović, Nikola Cvjetićanin, Srečo D. Škapin, Božidar Cekić, Valentin Ivanovski, Dragan Uskoković, "Preparation of LiFePO<sub>4</sub>/C composites by co-precipitation in molten stearic acid", *J. power sources*, vol. 196, no. 10, pp. 4613-4618, 2011.
- Marta Kasunič, Anton Meden, Srečo D. Škapin, Danilo Suvorov, Amalija Golobič, "Structure of LaTi<sub>2</sub>Al<sub>9</sub>O<sub>19</sub> and reanalysis of the crystal structure of La<sub>3</sub>Ti<sub>5</sub>Al<sub>15</sub>O<sub>37</sub>", *Acta crystallogr., B Struct. sci.*, vol. B67, no. 6, pp. 455-460, 2011.

- Prof. Malgorzata Jakubowska, Institute of Electronic Materials Technology, Warsaw, Poland, 21–22 November 2011
- Prof. Heli Jantunen, Dr. Jari Juuti, Dr. Merja Teirikangas, University of Oulu, Oulu, Finland, 21–22 November 2011
- 20. Dr. Juha Kuusisaari, Sachtleben Pigments Oy, Finland, 21-22 November 2011
- Prof. Velimir Radmilović, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Republic of Serbia, 1–3 December 2011
- 22. Mag. Peter Bastl, Mag. Vladimir Vrečko, Cinkarna Celje, Celje, 2 December 2011
- Hermann Gruenbichler, B. Sc., Dr. Manfred Schweinzger, Yongli Wang, B. Sc., TDK EPCOS, Deutschlandsberg, Austria, 22 December 2011

#### Visiting Researchers:

- Dr. Marija Vukomanović, Institute of Technical Sciences, SASA, Belgrade, Republic of Serbia, 1 January to 30 September 2011
- Dr. Ismael Fabregas, Centro de Investigaciones en Sólidos, CITEFA, Buenos Aires, Argentina, 12 October to 31 August 2012
- Sonja Jovanović, B. Sc.
   Dejan Klement, B. Sc.
   Mojca Otoničar, B. Sc.
   Andreja Šestan, B. Sc.
   Tina Šetinc, B. Sc.
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- 22. Slivo Zupancic

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- Varužan Kevorkijan, Uroš Kovačec, Irena Paulin, Srečo D. Škapin, Monika Jenko, "Modelling and preparation of core foamed Al panels with accumulative hot-roll bonded precursors", *Mater. tehnol.*, vol. 45, no. 6, pp. 537-544, 2011.
- Varužan Kevorkijan, Srečo D. Škapin, "Preparation and testing of prototype Mg<sub>2</sub>Si – Mg – TiC and Mg<sub>2</sub>Si – TiC/TiB<sub>2</sub> composites", *Mater. manuf. process.*, vol. 26, iss. 4, pp. 592-598, 2011.
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- Jakob Koenig, Matjaž Spreitzer, Danilo Suvorov, "Influence of the synthesis conditions on the dielectric properties in the Bi<sub>0.5</sub>Na<sub>0.5</sub>TiO<sub>3</sub> – KTaO<sub>3</sub> system", *J. Eur. Ceram. Soc.*, vol. 31, no. 11, pp. 1987-1995, 2011.
- 14. Ai Komatsu, Takuya Hoshina, Špela Kunej, Hiroaki Takeda, Takaaki Tsurumi, "Fabrication of BaTiO<sub>3</sub> films on Si substrate by inkjet printing", In: Electroceramics in Japan XIV: proceedings of the 30th Electronics Division Meeting, Tokyo, Japan, *Key Eng. Mater.*, vol. 485, pp. 187-190, 2011.
- Miodrag Lukić, Z. Stojanović, Srečo D. Škapin, Marjeta Maček, Miodrag Mitrić, Smilja Marković, Dragan Uskoković, "Dense fine-grained biphasic calcium phosphate (BCP) bioceramics designed by two-step sintering", *J. Eur. Ceram. Soc.*, vol. 31, no. 1, pp. 19-27, 2011.
   Marjeta Maček, Urban Došler, Danilo Suvorov, "The nucleation and
- Marjeta Maček, Urban Došler, Danilo Suvorov, "The nucleation and crystallization of Mg0 – B<sub>2</sub>O<sub>3</sub> – SiO<sub>2</sub> glass", *J. Eur. Ceram. Soc.*, vol. 31, no. 13, pp. 2211-2219, 2011.

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combination with hydroxyapatite to form composites via a sonochemical approach", *Cryst. growth des.*, vol. 11, issue 9, pp. 3802-3812, 2011.

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- 39. Vojka Žunič, Srečo D. Škapin, Marjeta Maček, Ines Bračko, Andrijana Sever Škapin, Danilo Suvorov, "Influence of the triblock copolymer P123 and phosphorous on the physico-chemical properties of TiO<sub>2</sub>", *Appl. catal., A Gen.*, vol. 397, no. 1/2, pp. 241-249, 2011.

## PUBLISHED CONFERENCE PAPERS

#### Regular papers

- Ines Bračko, Manca Logar, Boštjan Jančar, Danilo Suvorov, "Cu decorated titanate nanobelts composite thin film for photo-catalytic applications", In: *Nanotechnology 2011: conference and workshops, November 1-3, 2011, New York, NY*, [S. l., s. n.], 2011, pp. 55-56.
- 2. Varužan Kevorkijan, Uroš Kovačec, Irena Paulin, Srečo D. Škapin, Monika Jenko, "Izdelava Al pen in panelov na osnovi večstopenjsko toplo valjanih prekurzorjev", In: *Slovenski kemijski dnevi 2011, Portorož, 14-16 september 2011*, Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2011, 15 pp.
- 3. Tina Šetinc, Špela Kunej, Matjaž Spreitzer, Danilo Suvorov, "Influence of process parameters on the morphology and properties of CSD-derived SrTiO<sub>3</sub> thin films", In: *Nanotechnology 2011: conference and workshops, November 1-3, 2011, New York, NY*, [S. l., s. n.], 2011, pp. 50-51.
- 4. Erika Švara Fabjan, Andrijana Sever Škapin, Mojca Otoničar, Miran Gaberšček, "Encapsulation of nano-dimensional organic pigments by silica", In: *Conference proceedings*, 4th International Conference on Advanced Plasma Technologies (iCAPT-IV) with Workshop on Plasma Synthesis and Applications of Nanomaterials & 112th IUVSTA Executive Council Meeting, September 9th [i. e.] 11th - September 13th 2011, Strunjan, Slovenia, Miran Mozetič, ed., Uroš Cvelbar, ed., Ljubljana, Slovenian Society for Vacuum Technique, = DVTS - Društvo za vakuumsko tehniko Slovenije, 2011, pp. 193-197.
- 5. Erika Švara, Andrijana Sever Škapin, Luka Škrlep, Miran Gaberšček, Mojca Otoničar, "Determination of encapsulated organic pigments by electron microscopy", In: *e-Proceedings with full papers*, 13th Euroseminar on Microscopy Applied to Building Materials, Ljubljana, 14-18 June 2011, Alenka Mauko, ed., Tadeja Kosec, ed., Tinkara Kopar, ed., Nina Gartner, ed., Ljubljana, ZAG, = Slovenian National Building and Civil Engineering Institute, 2011, [7] pp.

## THESES

#### Ph. D. Thesis

1. Urban Došler, *The synthesis and characterization of glass-ceramic based on ternary system MgO-B<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>: doctoral dissertation, Ljubljana, [U. Došler], 2011.* 

## B. Sc. Thesis

<sup>1.</sup> Dejan Klement, *Influence of synthesis conditions on the structural and electrical properties of the Ag(Nb1-xTax)O3 ceramic:* undergraduate thesis, Ljubljana, [D. Klement], 2011.

# 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.

Proteases, which were long considered as primarily protein-degrading enzymes, are extremely important signalling molecules involved in numerous vital processes, such as cell-cycle regulation, proliferation, cell death and immune response. 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.

The tumour micro-environment regulates tumour progression and the spread of cancer in the body. Targeting the stromal cells that surround cancer cells could, therefore, improve the effectiveness of existing cancer treatments. And in this area we made a major achievement by developing a novel ferri-liposome-based targeted delivery system, which was published in Nature Nanotechnology - the first Slovenian paper ever published in this Head: journal. Using magnetic nanoparticle clusters encapsulated inside a liposome we have demonstrated that under Prof. Boris Turk the influence of an external magnet, the targeting of both the tumour and its micro-environment can be achieved. Moreover, we have used the outstanding T<sub>2</sub> contrast properties ( $r_2$ =573-1286 s(<sup>-1</sup>) mM(<sup>-1</sup>)) of these ferri-liposomes, which are ~95 nm in diameter, to non-invasively monitor drug delivery in vivo. We also visualized the targeting of the tumour microenvironment by the drug-loaded ferri-liposomes and the uptake of a model probe by cells. Furthermore, we used the ferri-liposomes to deliver a well-known, anticancer drug, doxorubicin, to a mammary tumour and its micro-environment in a mouse, which substantially reduced the size of the tumour compared with a systemic delivery of the same drug. Finally, using the same system we successfully delivered to the tumour site a broad-spectrum cathepsin inhibitor JPM-565, which was shown to be ineffective in the same mouse model due to poor bioavailability. As a consequence, the inhibitor successfully delayed the tumour growth, thereby also validating the cathepsins as drug targets for cancer treatment. To conclude, we have developed a universal drug-delivery system that can simultaneously allow drug delivery as well as the non-invasive in-vivo monitoring of drug delivery. Another work linked with cancer progression and the cathepsins was performed in collaboration with the group of prof. Janko Kos. Although it is known that aberrant cathepsin B activity is associated with tumour progression, there are no cathepsin B inhibitors in clinical use. In this work nitroxoline, an established antimicrobial agent, was identified as a potent, reversible inhibitor of cathepsin B, and thus a potential drug candidate for the treatment of cancer and also other diseases in which cathepsin B activity plays a role. The structure of the cathepsin B-nitroxoline complex was also determined to 2.11 Å.

We have also continued our work in the apoptosis field. It is well established that a major feature of apoptotic cell death is gross structural changes, one of which is the loss of cell-cell contacts. The caspases, executioners of apoptosis, were shown to cleave several proteins involved in the formation of cell junctions. The membrane-associated guanylate kinases (MAGUKs), which are typically associated with cell junctions, have a major role in the organization of protein-protein complexes at plasma membranes, and were therefore investigated as potentially important protease targets during apoptosis. We have demonstrated that MAGUKs are indeed cleaved and/or degraded by executioner caspases, granzyme B and several cysteine cathepsins in vitro. When apoptosis was induced by UV-irradiation and staurosporine in different epithelial cell lines, caspases were found to efficiently cleave MAGUKs in these cell models, as the cleavages could be prevented by a pan-caspase inhibitor N-benzyloxycarbonyl-Val-Ala-Asp(OMe) fluoromethylketone. Using a selective lysosomal disrupting agent L-leucyl-L-leucine methyl ester (LeuLeuOMe), which induces apoptosis through the lysosomal pathway, it was further shown that MAGUKs are also cleaved by the cathepsins in HaCaT and CaCo-2 cells. Immunohistological data showed the rapid loss of MAGUKs at the sites of cell-cell contacts, preceding actual cell detachment, suggesting that the cleavage of MAGUKs is an important step in fast and efficient cell detachment. In collaboration with prof. Gunnar Pejler, we have also extended our studies on the mechanism of LeuLeuOMe-induced cell death to mast cells. Mast-cell secretory granules (secretory lysosomes) contain large amounts of fully active proteases bound to serglycin proteoglycan. Damage to the granule membrane is therefore expected to lead to the release of serglycin and serglycin-bound proteases into the cytosol, which could potentially lead to proteolytic activation of cytosolic pro-apoptotic compounds. We showed that wild-type mast cells are highly sensitive to apoptosis induced by granule permeabilization, whereas serglycin-deficient cells are



largely resistant. The reduced sensitivity of serglycin(-/-) cells to apoptosis was accompanied by reduced granule damage, the reduced release of proteases into the cytosol, and defective caspase-3 activation. Mechanistically, the apoptosis-promoting effect of serglycin involved serglycin-dependent proteases, as indicated by reduced sensitivity to apoptosis and reduced caspase-3 activation in cells lacking individual mast cell-specific proteases. Together, these findings implicate serglycin proteoglycan as a novel player in mast-cell apoptosis.



Figure 1: Targeted delivery of a cysteine cathepsin inhibitor Jpm-565 using the novel ferriliposome-based delivery system significantly improved its bioavailability and consequently delayed the tumor growth.

We have also continued our work on protease inhibitors, in particular the members of the cystatin family. Stefin B (cystatin B) is an endogenous inhibitor of cysteine proteinases localized in the nucleus and the cytosol. Lossof-Function mutations in the stefin B (CSTB) gene were reported in patients with Unverricht-Lundborg disease (EPM1). In recent years, research into the molecular bases of neurodegenerative diseases has progressed, and therapies have been developed to combat the causative agents. Based on the observation that progressive myoclonus epilepsies (PMEs) and neurodegenerative diseases share common features of neurodegeneration, we propose that the two pathologies share common underlying molecular characteristics. It is well documented that autophagy is overloaded or impaired in neurodegenerative conditions, and it is also impaired in some PMEs, the clearest example being EPM2 (Lafora disease). Although more research into this connection is needed, we proposed that existing therapies for PMEs could be augmented with similar drugs as those used for neurodegenerative diseases. In addition, we continued our work on understanding the links between protein folding

and aggregation. The role of the aromatic residue at site 75 to protein stability, the mechanism of folding and the mechanism of amyloid-fibril formation were investigated for the human stefin B variant (bearing Y at site 31) and its point mutation H75W. In contrast to the wild-type protein, the mutant H75W did not fold to completion, ending in intermediate states at all the pH values studied, suggesting that an aromatic residue at position 75 is critical for the stability of the protein.

It is also well established that contact order and folding rates are correlated for small proteins. The folding rates of stefins A and B differ by nearly two orders of magnitude, despite sharing an identical native fold and hence contact order. In collaboration with Prof. Jonathan Waltho and dr. Rosemary Staniforth, we broke down the determinants of this behaviour and demonstrated that the modulation of contact-order effects can be accounted for by the combined contributions of a framework-like mechanism, characterized by intrinsic helix stabilities, together with a non-native helical backbone conformation and non-native hydrophobic interactions within the folding transition state. These contributions result in the formation of non-native interactions in the transition state, as evidenced by the opposing effects on the folding rate and the stability of these proteins.

In addition, we also expressed and characterized the human-blood plasma glutamate carboxypeptidase (PGCP), a protease that acts on the unsubstituted N- and C-termini of dipeptides. The recombinant human enzyme was purified as an active enzyme in the dimer form and as inactive precursor protein. The dipeptidase activity was confirmed by measuring the hydrolysis of the Ser-Met dipeptide at a slightly acidic pH. Finally, we also collaborated with other groups from the Institute in nanoparticle characterization.

We participate in two FP7 projects, and are 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 many other international collaborations with excellent research teams from different countries, including Belgium, Germany, France, Sweden, Switzerland, UK, USA, Australia and Japan, which resulted in joint publications. For his work Prof. Boris Turk received the Zois Award for Outstanding Achievements in Science for his work on signal transduction by proteases, and was, at the 7<sup>th</sup> General Meeting of the International Proteolysis Society in San Diego in October 2011, elected as the President of the Society for the next two years. Several members of the department were invited to give lectures at international symposia and foreign universities.

#### Some outstanding publications in 2011:

- Mikhaylov, G. Mikac, U., Magaeva, A.A., Itin, V.I., Naiden, E.P., Psakhye, I., Babes, L., Reinheckel, T., Peters, C., Zeiser, R., Bogyo, M., Turk, V., Psakhye, S.G., Turk, B., Vasiljeva, O. (2011) Nanosized ferri-liposomes: a novel MRI-visible drug delivery system for targeting tumours and their microenvironment, Nat. Nanotech. 6, 594-602.
- Polajnar, M., Žerovnik, E.. Impaired autophagy : a link between neurodegenerative diseases and progressive myoclonus epilepsies. Trends Mol. Med. (Print), 2011, 17, 293-299.

- Ivanova S, Gregorc U, Vidergar N, Javier R, Bredt DS, Vandenabeele P, Pardo J, Simon MM, Turk V, Banks L, Turk B. (2011) MAGUKs, scaffolding proteins at cell junctions, are substrates of different proteases during apoptosis. Cell Death Dis. 2:e116.
- Jelinska, Clare, Davis, Peter J., Kenig, Manca, Žerovnik, Eva, Kokalj-Jenko, Saša, Gunčar, Gregor, Turk, Dušan, Turk, Vito, Clarke, David T., Waltho, Jonathan P., Staniforth, Rosemary A. Modulation of contact order effects in the two-state folding of stefins A and B. Biophys. J., 2011, 100, 2268-2274.

#### Awards and appointments

1. Boris Turk, Presented with the Zois Award for highest scientific research contributions in the field of transmission of signals with proteases.

## Organization of conferences, congress and meetings

1. 28<sup>th</sup> Winter School on Proteinases and their Inhibitors, Recent Developments, Tiers, Italy, 23 to 27 Feb. 2011 (co-organisers)

# INTERNATIONAL PROJECTS

- 1. Light-based Functional in Vivo Monitoring of Diseases Related Enzymes LIVIMODE
  - 7. FP
  - 241919
  - EC
- Prof. Boris Turk, Prof. Vito Turk, Dr. Urška Repnik, Asst. Prof. Marko Fonovič Understanding and Fighting Metastasis by Modulating the Tumour Microenvironment
- 2. Onderstanding and righting increasiants by modulating the runnour increase through Interference with the Protease Network MICROENVIMET
  - 7. FP
  - 201279
  - EC; Universite de Liege, Liege, Belgium
  - Asst. Prof. Olga Vasiljeva, Prof. Boris Turk
- Function of Proteases in TRAIL/DR5-induced Apoptosis Pathway BI-CN/09-11-006

Dr. Juan Shi, National Laboratory of Medical Molecular Biology, Institute of Basic Medical Sciences, Chinese Academy of Medical Sciences & Peking Union Medical College, Beijing, China Prof. Boris Turk

- 4. The Role of Cysteine Proteinases and Their Inhibitors in Endotoxin Tolerance and Cancer
  - BI-CN/09-11-024

Dr. Tao Sun, Liaoning Cancer Hospital & Institute, Shanghai, China Asst. Prof. Nataša Kopitar Jerala

# R & D GRANTS AND CONTRACTS

- 1. Proteomic identification of extracellular substrates of cysteine proteases
- Asst. Prof. Marko Fonović 2. Role of cysteine cathepsins in regulation of proliferation and cell death Dr. Boris Turk
- Differences between mouse and human endosomal immune response pathway:Crystal structures of protein comlexes and their analysisProf. Dušan Turk
- Cathepsin E: characterisation and biological role Prof. Vito Turk
- The role opf lysosomes and lysosomal proteases in cellular signalling Prof. Boris Turk
- 6. The role of cysteine cathepsins in cellular signalling Asst. Prof. Boris Turk

# MENTORING

## Ph. D. Thesis

 Katja Škerget, Contribution to understanding of the mechanism of amyloid fibril formation and its effects on the cell (mentor Eva Žerovnik; co-mentor Uroš Petrovič).

- 7. Cell signalling of Toll-like receptors Asst. Prof. Nataša Kopitar - Jerala
- Role and relevance of empirical geometric parameters in crystal structure determination of macromolecules for prediction of ligand binding Prof. Dušan Turk
- 9. The role of nuclear cystatins in the regulation of interleukin-10 synthesis during endotoxin tolerance
- Asst. Prof. Nataša Kopitar Jerala 10. The role of cysteine cathepsins and caspases in neurodegeneration Prof. Veronika Stoka
- The role of small GTPases in the regulation of endosomal/lysosomal transport in astrocytes
- Prof. Igor Mekjavić 12. Secretory vesicle mobility and calcium homeostasis in astrocytes Prof. Veronika Stoka
- 13. Involvement of the Lysosomal Cysteine Peptidase Inhibitors in Progression and Metastasis of Mammary Cancer
- Asst. Prof. Olga Vasiljeva 14. Inhibitors of cysteine carboxypeptidases as regulators of autoimmune and neurodegenerative processes Prof. Janko Kos
- Study of hom(e)ologous recombination in the evolution of polyketide synthases Prof. Boris Turk
- 16. Oligomers of amyloidogenic proteins from a to z: biophysical properties, structure, function and mutual interactions
- Prof. Eva Žerovnik 17. New biotechnological drugs obtained by phage display
- Prof. Borut Štrukelj
  18. Research on new technologies for conservation restoration of baroque easel paintings Asst. Prof. Marko Fonović

# **RESEARCH PROGRAMS**

- 1. Structural biology
- Prof. Dušan Turk 2. Proteolysis and its regulation
- 2. Proteolysis and its regula Prof. Boris Turk

# VISITORS FROM ABROAD

- Georgy Mikhaylov, Siberian State Medical University, Tomsk, Siberia, 1 Jan.-31 Dec. 2011, (Scholarship IJS)
- dr. Igor Vilfan, NGAT group, Pacific Biosciences, Menlo Park, CA 94025, USA, 12 Sept. 2011
- 3. dr. Luca Scorrano, University of Genève, Switzerland, 13 Oct. 2011
- prof.dr. Kazuo Umezawa, Keio University, Faculty of Science and Technology, Yokohama, Japan, 6.-8. Nov. 2011

# STAFF

#### Researchers Dr. Iztok Dolenc 1. Asst. Prof. Marko Fonović 2 Asst. Prof. Nataša Kopitar - Jerala 3. 4. Prof. Brigita Lenarčič' Asst. Prof. Urška Repnik 5. 6 Prof. Veronika Stoka Andrej Šali, B. Sc. 8. Prof. Boris Turk, Head Prof. Dušan Turk 10. Prof. Vito Turk 11. Dr. Livija Tušar 12. Asst. Prof. Olga Vasiljeva 13. Dr. Tina Zavašnik Bergant 14. Prof. Eva Žerovnik Postdoctorial associates 15. Dr. Dejan Caglič, left 22.05.11 16. Dr. Katarina Črnigoj Kristan 17. Dr. Saška Ivanova 18. Dr. Marko Mihelič 19. Dr. Katarina Pegan 20. Dr. Ana Petelin, left 01.10.11 21. Dr. Cristina Gabriela Pinto Droga Mazovec 22. Dr. Mojca Podlesnik Beseničar, left 01.07.11 23. Dr. Jure Pražnikar' 24. Dr. Miha Renko 25. Dr. Aleksandra Usenik Postgraduates 26. Katja Bidovec, B. Sc.

27. Miha Butinar, B. Sc. 28. Maruša Hafner Česen, B. Sc. 29. Barbara Jerič, B. Sc. 30. Katarina Maher, B. Sc. 31. Mira Polajnar, B. Sc. 32. Jelena Rajković, B. Sc. 33. Barbara Sobotič, B. Sc. 34. Dejan Suban, B. Sc. 35. Aleš Špes, B. Sc. 36. Ajda Taler-Verčič, B. Sc. 37. Mojca Trstenjak Prebanda, B. Sc. 38. Nina Vidergar, B. Sc., left 01.02.11 39. Robert Vidmar, B. Sc. 40. Matej Vizovišek, B. Sc. 41. Tajana Zajc, B. Sc. 42. Janja Završnik, B. Sc. **Technical officers** 43. Andrejka Doberšek, B. Sc. 44. Vida Puizdar, M. Sc. 45. Andreja Sekirnik, B. Sc. 46. Ivica Štefe, B. Sc. Technical and administrative staff 47. Louisa Johanna Kroon Žitko, B. Sc. 48. Dejan Pelko 49. Polonca Pirš Kovačič 50. Barbara Vrtačnik

Note: \* part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLES

- 1. Ines Bračko, Boštjan Jančar, Manca Logar, Dejan Caglič, Danilo Suvorov, "Silver nanoparticles on titanate nanobelts via the selfassembly of weak polyelectrolytes: synthesis and photocatalytic properties", *Nanotechnology (Bristol)*, vol. 22, issue 8, pp. 085705-1-085705-11, 2011.
- 2. Dejan Caglič *et al.* (11 authors), "Functional in vivo imaging of cysteine cathepsin activity in murine model of inflammation", *Bioorg. med. chem.*, vol. 19, issue 3, pp. 1055-1061, 2011.
- 3. Kristina Eleršič, Ita Junkar, Aleš Špes, Danijela Vujošević, Zoran Vratnica, Uroš Cvelbar, "Etching of bacterial capsule and cell wall by oxygen plasma afterflow", *IEEE trans. plasma sci.*, vol. 39, no. 11, part 1, pp. 2972-2973, 2011.
- 4. Saška Ivanova, Uroš Gregorc, Nina Vidergar, Ron Javier, David S. Bredt, Peter Vandenabeele, J. Pardo, Markus M. Simon, Vito Turk, Lawrence Banks, Boris Turk, "MAGUKs, scaffolding proteins at cell junctions, are substrates of different proteases during apoptosis", *Cell death & disease*, vol. 2, pp. e116-1-e116-11, 2011.
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## **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

- 1. Michael Duszenko *et al.* (18 authors), "Autophagy in protists", *Autophagy*, vol. 7, no. 2, pp. 127-158, 2011.
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## PUBLISHED CONFERENCE PAPERS

#### **Invited** Paper

1. Dušan Turk, "Proteini - nosilci življenja", In: *Povezanost procesov: zbornik prispevkov: proceedings*, Mednarodni posvet Biološka znanost in družba, Ljubljana, 6. in 7. oktober 2011 = Conference on Bioscience and Society, October 6-7, 2010, Ljubljana, Slovenia, Minka Vičar, ed., Saša Kregar, ed., Frances M. Ashcroft, 1. izd., Ljubljana, Zavod RS za šolstvo, 2011, pp. 25-28, 2011.

#### Regular paper

1. Veronika Stoka, Vito Turk, "Strukturna in funkcijska mreža kot orodje za razvoj učinkovitejših pristopov vosebni terapiji", In: *Osebna genomika med medicinsko uporabo in komercializacijo: zbornik*  *povzetkov*, 3. Simpozij slovenske medicinske genetike = 3rd Slovene Medical Genetics Symposium, Ljubljana, 8. aprila 2011, Luca Lovrečić, ed., Nataša Teran, ed., Ljubljana, Združenje za medicinsko genetiko, Slovensko zdravniško društvo, 2011, pp. 37-39.

## TEXTBOOKS AND LECTURE NOTES

1. Eva Žerovnik, *Zvijanje in agregacija proteinov: uvodno predavanje,* Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 24. maj 2011.

## THESES

## Ph. D. Theses

- 1. Katarina Pegan, *The role of apoptosis in the regeneration of human skeletal muscle under in vitro conditions:* doctoral dissertation, Ljubljana, [K. Pegan], 2011.
- Aleksandra Usenik, Izražanje nativnega in mutiranih genov 6fosfofrukto-1-kinaze glive Aspergillus niger v bakteriji Escherichia coli in kvasovki Saccharomyces cerevisiae: doctoral dissertation, Ljubljana, [A. Usenik], 2011.
# DEPARTMENT OF MOLECULAR AND **BIOMEDICAL SCIENCES** R-2

The research program of the Department of Molecular and Biomedical Sciences is focused mainly 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 topics of the department are sPLA<sub>s</sub>s originating from animal toxins as well as those found in humans. We are studying the molecular mechanisms of the action of toxic sPLA, s, particularly those endowed with presynaptic neurotoxicity, and the role of endogenous sPLA, s in pathological and physiological processes in mammals.

In the past year the most intensive research has been performed in the area of the molecular mechanism of the action of presynaptically neurotoxic sPLA, s. As the model sPLA, in these studies we used ammodytoxin (Atx) from the venom of the nose-horned viper (Vipera ammodytes ammodytes). With particular intensity we have been trying to find answers about the identity of the specific Atx receptor in the presynaptic membrane of the motoneuron, Prof. Igor Križaj the so-called N-type sPLA, receptor, and about intracellular events following translocation of the toxin through the neuronal plasma membrane. In the N-type sPLA, receptor studies we joined forces on a bilateral project Proteus with the renowned group from the Institute for Molecular and Cellular Pharmacology CNRS (Institut de Pharmacologie Moléculaire et Cellulaire CNRS) from Valbonne, France. By the means of protein engineering and chemical synthesis we almost finished the preparation of molecular tools to dynamically follow the localization of Atx in cells and its interactions with binding proteins. Calmodulin (CaM) is one of the binding proteins of Atx in the cytosol of the nerve cell. Complexed to CaM, Atx becomes completely stable in a reducing environment, such as the cytosol, and

its enzymatic activity substantially increases. Why such pathophysiologically potentially very important effects occur we started to study within the scope of a new postdoctoral project. Using the recombinant DNA technology, we prepared in 2011 isotope-labelled Atx and CaM, which we need to study the



interactions between these two proteins and interactions of the complex Atx-CaM with the phospholipid membrane by the nuclear magnetic resonance (NMR). Our partner groups in the NMR studies are prominent NMR centres: the Bijvoet Centre from Utrecht University, Netherlands, and the centre from the National Institute of Chemistry, Ljubljana, Slovenia. In the bilateral project with Bulgarian colleagues from the Sofia University, we discovered differences in the mechanism of the neurotoxic action of monomeric Atx from the venom of our subspecies of the

nose-horned viper (V. a. ammodytes) and the two-chain vipoxin from the venom of a Bulgarian subspecies of the snake (V. a. meridionalis). Interestingly, in spite of the high structural identity between Atx and vipoxin, the mechanisms of their neurotoxic action differ substantially.

Very important steps in searching for the answer about the mode of action of this group of lethal neurotoxins have been made by using Atx. Invited by the Editor of Toxicon, a leading journal in the field of toxinology, the review article, describing comprehensively experiments performed on Atx and with Atx, was prepared (I. Križaj, Toxicon, 58 (2011) 219-229). This article was an introductory one into a new series of review articles, Classic Toxins Review, in Toxicon, which we considered as a special recognition of the achievements of our group. In a review article we presented the results of our past and latest research about the relationships between the structure and the function of neuro- and myotoxic sPLA,s from the venom of the nose-horned viper (J. Pungerčar et al., Acta Chimica Slovenica, 58 (2011), 660-670).

Our studies on the involvement of endogenous mammalian sPLA,s in breast cancer were continued in 2011. Ten structurally distinct sPLA, enzymes are known in humans displaying diverse roles in a variety of physiological and pathophysiological processes owing to their enzymatic action on cellular and non-cellular phospholipids, the downstream effects of the products at 100-times magnification.

### New substances and molecular tools to improve human and animal health.



Figure 1: Immunofluorescently labelled sPLA<sub>2</sub>-X, transiently expressed in breast-cancer cells MDA-MB-231. Cell nuclei stained by a blue fluorescence dye. Green punctuate fluorescence stems from sPLA<sub>2</sub>-X in the cytoplasm. The photograph was taken using epifluorescence microscope



Figure 2: Cell-death analysis by flow cytometry following the exposure of the breast-cancer MDA-MB-231 cells to a nanomolar concentration of recombinant sPLA<sub>2</sub>X. Viable cells (bottom left), cells in the early apoptotic phase (bottom right), cells in the late apoptotic phase (top right) and necrotic cells (top left).

of their hydrolysis or due to interactions with specific binding proteins. In mammals, sPLA<sub>2</sub>s are involved in lipid digestion and homeostasis, inflammatory and immune response, acute and chronic airway disorders, atheroscle-rosis, host defence against infections, and recently they have also been implicated in cell proliferation, apoptosis

and cancer. Due to their very low phospholipid-head group and acyl-chain specificity, their diverse tissue and cell expression patterns, and their ability to act intra- and extracellularly, they often display, apparently, contradictory biological roles, e.g., cell-growth promotion or inhibition. Indeed, we have previously shown that a particular sPLA, may induce cell proliferation, apoptosis and neurotoxicity in different cellular environments. Recent studies have associated the expression of several sPLA,s with the pathology of colorectal and prostate cancers, with roles in either tumour promotion or inhibition, depending on the tissue and the biochemical microenvironment of the tumour involved. Their involvement in cancer biology might be related to their role in liberating arachidonic acid (AA) and lysophospholipids, such as lysophosphatidylcholine (LPC), from membrane phospholipids, which influence cell proliferation, survival and angiogenesis. AA is an important substrate for intracellular biochemical pathways that generate eicosanoids, potent autocrine and paracrine lipid mediators, including the mitogenic prostaglandins (PGs), which have been associated with a number of malignancies, including breast cancer. On the other hand, LPC can be converted to lysophosphatidic acid (LPA), which is a potent lipid mediator known to induce cell proliferation, survival and migration, critical requirements for cancer progression. Additionally, the elevated expression of several important enzymes involved in eicosanoid metabolism, including cyclooxygenase-2 (COX-2) that catalyses the first step of AA conversion to various PGs, is a hallmark of different malignancies, including colorectal, prostate and breast cancer. However, the clinical use of non-steroidal anti-inflammatory drugs (NSAIDs) including specific COX-2 inhibitors in cancer prevention and

treatment, as well as in pain and inflammation relief, is associated with some seriously adverse effects. Therefore, considering their importance in regulating the availability of AA and lysophospholipids for downstream biosynthetic pathways that produce a variety of important lipid mediators, which influence the crucial determinants of cancer initiation and progression, sPLA, s are promising new targets for cancer prevention and therapy.



Figure 3: Secreted PLA<sub>2</sub>s interact with a plethora of structurally different proteins. Some of these, containing well-defined structural motifs, are shown. CRD: carbohydrate recognition domain; Ig: immunoglobulin; LRR: leucine-rich repeat. The figure is reproduced from J. Šribar in I. Križaj, Acta Chimica Slovenica, 58 (2011), 678–688.

In our recent initial study of the involvement of sPLA, s in breast cancer, we have determined the expression profile of all the sPLA, family members in human breast-cancer cell models representing different stages in the progression of the disease. Using a validated method for the quantitative PCR expression analysis of the whole set of human sPLA<sub>s</sub>, we identified several differentially expressed sPLA<sub>s</sub> in breast-cancer cells, namely the group IIA, III, V and X enzymes. For example, the group IIA sPLA, was overexpressed in moderately to highly invasive cell lines, while the group X enzyme (sPLA<sub>2</sub>-X) was overexpressed in weakly and moderately invasive cells, but its expression was not detected in highly invasive and tumourigenic cell lines. In our latest studies in 2011, we have found that the expression of some sPLA<sub>s</sub> is upregulated by inflammatory cytokines, such as IL1 $\beta$  and TNF $\alpha$ , in breast cancer cells. Furthermore, the treatment of cells with a DNA demethylating agent resulted in a significant increase in the expression of several sPLA, isoforms, indicating that the regulation of sPLA<sub>2</sub>s in breast cancer involves epigenetic silencing by DNA hypermethylation. The differential expression patterns of sPLA<sub>2</sub>s, the regulation by inflammatory cytokines and the epigenetic silencing suggest a potential role for these enzymes in human breast cancer and indicate that different sPLA,s may have distinct roles at different levels of progression of the disease. Indeed, our gain-of-function studies, performed by ectopically overexpressing sPLA2-X in the highly invasive cell line MDA-MB-231 (Figure 1), show that the enzyme promotes breast-cancer cell survival by increasing

their proliferation rate and viability. A similar effect was observed after the exogenous addition of low nanomolar concentrations of recombinant sPLA<sub>2</sub>-X to the highly invasive breast-cancer cells. Interestingly, sPLA<sub>2</sub>-X also reduced the level of spontaneous apoptosis *in vitro* (Figure 2), suggesting a novel role for sPLA<sub>2</sub>-X in promoting breast-cancer

cell survival. Therefore, our results focused on the regulation of sPLA, expression and their influence on breast-cancer cell growth are very promising and suggest a novel protumourigenic role for the group X sPLA,, which might be a consequence of the different mechanisms of action affecting apoptosis and cell proliferation.

In the past year, in the research of the role of endogenous sPLA,s in the peripheral nervous system, we used cellular models of motor neurons to study the (intra)cellular localization of exogenously added human sPLA,-X and snake presynaptically neurotoxic sPLA,, ammodytoxin A (AtxA). In the context of these studies, we first prepared the recombinant cysteine mutants with a single-site substitution N79C in the molecules of both sPLA<sub>2</sub>s that were

subsequently directly tagged with a fluorescent marker. The latter were exogenously added to the cell media and we monitored their internalization into a cell line of mouse motor neurons and into a heterologous tissue co-culture, prepared by explants of rat embryonic spinal cord and human skeletal (striated) muscle cells. We found that AtxA entered the mouse motoneuronal cells using the internalization pathway of human sPLA,-X, although their intracellular colocalization with mitochondria and lysosomes showed certain important differences between the two sPLA,s. The results were compared with those obtained in the tissue co-culture of rat spinal cord explants and human muscle cells, and again we encountered certain differences in the localization of both sPLA,s. A fluorescence microscopy analysis showed that after the addition the human sPLA,-X is located primarily in neurites, whereas AtxA is specifically localized to the neuromuscular junctions. To analyse the effect of sPLA<sub>2</sub>-X on the tissue co-culture, we treated the latter with different concentrations of sPLA<sub>2</sub>-X and monitored their effect on the formation of functional neuromuscular junctions in the heterologous co-culture. We found that the addition of sPLA,-X, depending on its concentration, has a significant influence on, i.e., modulates, the formation of neuromuscular junctions. A part of the results was obtained in collaboration with Dr. Tomaž Marš from the Institute for Pathophysiology, Medical Faculty, University of Ljubljana, Figure 4: Phylogenetic tree of the aD-conopeptides. The figure is and also presented at the international scientific conference SiNAPSA Neuroscience 2011 in Ljubljana.



reproduced from D. Mebs et al., Acta Chimica Slovenica, 58 (2011), 730-734.

In a review paper we presented a comprehensive overview of sPLA,

binding proteins (J. Šribar and I. Križaj, Acta Chimica Slovenica, 58 (2011), 678-688). Novel interactors of these proteins are progressively discovered and it has become evident that many pathophysiological actions of sPLA,s are linked not only to their enzymatic activity but also to their ligand function (Figure 3).

In the scope of a bilateral project with researchers from the Institute of Immunology in Zagreb, Croatia, we continued our efforts to prepare an efficient antiserum towards the nose-horned viper venom. We found that methods for the quantification of Atx content in the venom clearly differentiate between high and low immunogenic venoms of the nose-horned viper (B. Halassy et al., Comparative Biochemistry and Physiology, Part C, 153 (2011), 223–230).

### Other pharmacologically active components from natural toxins

In 2011 we continued the intensive study of the components of the nose-horned viper venom that affect the coagulation of blood - haemostasis. Within this topic we also published a comprehensive review article (T. Sajevic et al., Toxicon, 57 (2011), 627-645), which was the seventh most downloaded paper of the journal at the end of last year. We were able to obtain financing and started a new basic research project in 2011 in this area of our research. With our partners from the University Medical Centre Ljubljana, Division of Pediatrics, we evaluated the influence of venom fractions on different components of human haemostatic system. In collaboration with our colleagues from the Institute of Immunology in Zagreb, Croatia, we concluded part of our project by publishing a paper reporting on the characterisation of a potently hemorrhagic metalloprotease (MP) from the nose-horned viper venom, ammodytagin (T. Kurtović, et al., Toxicon, 58 (2011), 570-582). Ammodytagin represents the first dimeric MP described in this venom. A very important result described in this paper was that it is possible to completely neutralize the hemorrhagic activity of the whole venom by the antiserum raised only against ammodytagin. The preparation of a new cDNA library from the nose-horned viper venom glands has been initiated in 2011, the main goal of which was to isolate a full-length mRNA transcipt encoding ammodytase.

As one of the 20 partners on 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. At the beginning of 2011 we organized a very successful meeting of the project consortium at Brdo near Kranj.

Venoms of the marine cone snails consist of numerous proteins and peptides showing a wide variety of biological activities, such as their effects on ion channels and receptors. Conopeptides acting on neuronal nicotinic acetylcholine receptors (nAChRs) belong to several peptide superfamilies, including the recently described  $\alpha$ D-conopeptides, which are homodimers of identical peptides with 47–49 amino acids. It has been demonstrated that  $\alpha$ D-conopeptides specifically block the mammalian neuronal nAChRs of the  $\alpha$ 7,  $\alpha$ 3 $\beta$ 2 and  $\alpha$ 4 $\beta$ 2 subtypes in



Figure 5: A method to design a new generation strains of industrial microorganisms.

nanomolar concentrations. Among the venom glands of 27 Conus species analyzed by cDNA cloning, precursors of the  $\alpha$ D-conopeptides were identified in four species only: C. betulinus, C. capitaneus, C. mustelinus and C. vexillum. A phylogenetic analysis of the relationships among the  $\alpha$ D-conopeptides revealed that they belong to clades that are characterized by an AVV- and EMM-motif in the signal peptide sequence (Figure 4). The distribution of the  $\alpha$ D-conopeptides in the *Conus* species is very limited. The overall dominance of these peptides and the low abundance or even lack of small  $\alpha$ -conopeptides in the venoms of these *Conus* species may suggest that  $\alpha$ D-conopeptides are an adaptation to a specific type of prey, *i.e.*, marine worms (D. Mebs et al., Acta Chimica Slovenica, 58 (2011), 730-734). We performed phylogenetic and biogeographic analyses of diverse Indo-Pacific and endemic South African venomous cone snails (S. Kauferstein et al., Toxicon, 57 (2011), 28-34). The phylogenetic analysis of the 16S RNA from numerous Conus species has clarified the evolutionary position of the endemic South African Conus species and provided the first evidence of their close genetic relationship.

Experimentally, a comparative proteomic analysis of the high-molecularmass protein components in the cone snail venom duct and in its injected venom has been concluded. Some of our results are close to final acceptance

for publication in *Marine Drugs*, whereas the main part of the results is still in preparation for publication.

### 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. In 2011, we have brought to an end a landmark stage of our long-term studies of a protein called Pex11, which has an important role in the cellular processes linked to the metabolism of fats, but its molecular function was not known until our study. We have now discovered that Pex11 senses acetyl-CoA, a central molecule in the cellular energy metabolism, and transfers information to the level of the regulation of the expression of some genes that are crucial for energy metabolism. In addition, we have found a small molecule agonist of Pex11 that can modulate the regulation of the expression of the respective genes. These results represent an important step in our understanding of the cellular processes leading to obesity and type-2 diabetes, and provide a new avenue for finding a medical treatment for these conditions.

Quantitative trait is a term that describes the variability in the expression of a phenotypic trait that shows continuous variability, and is the net result of multiple genetic loci, called quantitative trait loci (QTLs). The majority of the economically important phenotypic traits in strains of industrial microorganisms are quantitative traits. In collaboration with our colleagues from the University of Graz, Austria, from the University of Toronto, Canada, and from the Faculty for Computer and Information Sciences of the University of Ljubljana, we have developed a method to identify QTLs in yeast at the level of a single allele, and the genetic interactions between them, in a quantitatively defined population of genetically different yeast strains. Subsequently, using established methods, the transfer of identified alleles into a yeast strain with a different allele version is then performed to generate a biotechnologically improved strain. This method provides a step towards a new approach for a knowledge-based and targeted design of industrial microbiological strains (Figure 5).

### Evolutionary genomics and study of retrotransposons

Early evolutionary analyses of sPLA<sub>2</sub> toxins in venomous animals took place in the 1990s, in the so-called "pre-genomic era", and were based on a small sample of taxonomic diversity and diversity within the sPLA<sub>2</sub> toxins. Since then, the number of representatives has increased significantly, largely due to the accumulation of the venom transcriptomic resources, since the large genomic data regarding sPLA<sub>2</sub> toxins in venomous animals are still very sparse. In an invited review (D. Kordiš, *Acta Chimica Slovenica*, 58 (2011), 638–646) we highlighted how the progress in the past decade has increased our understanding of the evolution of sPLA<sub>2</sub> toxins in venomous animals.

Genome-wide studies of the intron dynamics in mammalian orthologous genes have found convincing evidence for the loss of introns, but very little for intron turnover. Similarly, a large-scale analysis of intron dynamics in a few vertebrate genomes has identified only intron losses and no gains, indicating that intron gain is an extremely rare event in vertebrate evolution. These studies suggest that the intron-rich genomes of vertebrates do not allow intron gain. We searched for evidence of a *de novo* intron gain in domesticated genes from an analysis of their exon/intron structures. A phylogenomic approach has been used to analyse all the domesticated genes in mammals and chordates that originated from the coding regions of transposable elements (D. Kordiš, Biology Direct, 6-59 (2011)). The gain of introns in domesticated genes has been reconstructed on well-established mammalian, vertebrate and chordate phylogenies, and examined as to where and when the gain events occurred. The locations, sizes and amounts of *de novo* introns gained in the domesticated genes during the evolution of mammals and chordates have been analyzed. A significant amount of intron gain was found only in the domesticated genes of placental mammals, where more than 70 cases were identified. De novo gained introns show a clear positional bias, since they are distributed mainly in the 5'-UTR and coding regions, while the 3'-UTR introns are very rare. In the coding regions of some domesticated genes up to 8 de novo gained introns have been found. The intron densities in Eutheria-specific domesticated genes and in older domesticated genes that originated early in vertebrates are lower than those in "normal" mammalian and vertebrate genes (Figure 6). Surprisingly, the majority of intron gains have occurred in the ancestor of placentals. This study (D. Kordiš, Biology Direct, 6-59 (2011)) provides the first evidence for numerous intron gains in the ancestor of placental mammals and demonstrates that adequate taxon sampling is crucial for reconstructing intron evolution. The findings of this comprehensive study challenge the current view on the evolutionary stasis in intron dynamics during the last 100-200 My. Domesticated genes could constitute an excellent system for the analysis of the mechanisms of intron gain in placental mammals.

Efts and adult specimens of the red-spotted newt Notophthalmus viridescens from various locations in Canada and the USA were analyzed for the presence of tetrodotoxin (TTX) and of its analogues 6-epitetrodotoxin and 11-oxotetrodotoxin. Considerable individual variations in toxin levels were found within and among populations from New Hampshire, New York, Pennsylvania, and Virginia, ranging from nondetectable to 69µg TTX per gram of newt. TTX and its analogues were absent in efts and adults from various locations in the Canadian province of Nova Scotia, the northernmost distribution 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 analyses of the 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. An exogenous source of TTX in the newts either via the food chain or by synthesis of symbiotic bacteria is suggested to explain the high variability and lack of TTX in certain populations. A paper about this topic will be published next year.

In 2011 we collaborated with our colleagues from the Faculty of Chemistry and Chemical Technology, University of Ljubljana (UL), also on a new basic research project on how APOBEC3 proteins inhibit L2 retrotransposon multiplication. An explanation of the mechanism of action of APOBEC3



Figure 6: Intron densities in domesticated genes compared with vertebrate, mammalian and human "normal" genes. The figure is reproduced from D. Kordiš, Biology Direct, 6:59 (2011).

proteins is very important as these proteins block the proliferation of numerous retrotransposons and retroviruses, among them also HIV.

#### **Other subjects**

In 2011 we also collaborated in several projects out of the thematic scope of our department or the programme group "Toxins and biomembranes".

By analyzing the DNA and RNA samples from patients with unipolar depression we participated in a pharmacogenetic study of alternative antidepressant response of these people (K. Malki et al., *Biological Psychiatry*, 69 (2011), 360–365). With a structural analysis we participated in the identification of the cysteine protease inhibitor from the filamentous yeast *Trichophyton mentagrophytes* on the project from the Veterinary Faculty, UL (B. Premrov Bajuk et al., *Acta Chimica Slovenica*, 58 (2011), 33–40). We also structurally characterized lectins isolated from the basidomycete *Clitocybe nebularis* isolated by colleagues from the Department of Biochemistry, at the Jožef Stefan Institute (J. Pohleven et al., *Applied Microbiology and Biotechnology*, 91 (2011), 1141–1148). In the case of amyotrophic lateral sclerosis and TDP-43 proteinopathies, the TDP-43 protein localizes and aggregates in the cytosol rather than in the cell nucleus. We collaborated in the description of action of TDP-43 at the RNA level (J.R. Tollervey et al., *Nature Neuroscience*, 14 (2011), 452–458). In collaboration with the Utrecht University NMR centre, we participated in the development of an original protocol for the synthesis of a lanthanide tag for the paramagnetic labelling of proteins in NMR experiments (F. Peters et al., *Journal of Biomolecular NMR*, 51 (2011), 329–337). With the same group we also prepared a chapter in the monography "NMR of Biomolecules" that will be



Figure 7: Cover page of the fourth issue of Acta Chimica Slovenica 2011, dedicated to the memory of the late Professor Franc Gubenšek, one of the founders of toxinology in Slovenia.

published in 2012 by the publisher Wiley. In 2011 we also started a collaboration within the other two new basic research projects. With colleagues from the Biotechnical faculty, UL, we initiated research on the apoptotic effects of alkylpyridinium compounds on lung adenocarcinoma cells and changes of membrane lipid structure in the pathological state.

Two achievements of the department in 2011 worth mentioning are connected with the late Professor Franc Gubenšek. First, to commemorate his memory we organized a special section at the congress of the European Section of the International Society on Toxinology in Valencia, Spain. The section was very well attended and accepted. Second, we edited a special issue of the journal *Acta Chimica Slovenica* (Figure 7). In this issue some of the most prominent scientists in the field of toxinology contributed their papers.

### Some outstanding publications in the past year

- 1. Halassy, B., Brgles, M., Habjanec, L., Lang Balija, M., Kurtović, T., Marchetti Deschman, M., Križaj, I. and Allmaier, G. (2011): Intraspecies variability in *Vipera ammodytes ammodytes* venom related to its toxicity and immunogenic potential. *Comp. Biochem. Biophysiol. Part C* 153, 223–230.
- 2. Sajevic, T., Leonardi, A. and Križaj, I. (2011): Haemostatically active proteins in snake venoms. *Toxicon* 57, 627–645.
- 3. Kordiš, D. (2011): Extensive intron gain in the ancestor of placental mammals. *Biol. Direct* 6:59, doi:10.1186/1745-6150-6-59.

4. Tollervey, J.R., Curk, T., Rogelj, B., Briese, M., Cereda, M., Kayikci, M., König, J., Hortobágyi, T., Nishimura, A.L., Župunski, V., Patani, R., Chandran, S., Rot, G., Zupan, B., Shaw, C.E. and Ule, J.

(2011): Characterizing the RNA targets and position dependent splicing regulation by TDP-43. *Nat. Neurosci.* 14, 452–458.

5. Peters, F., Martinez, M.M., Leonov, A., Kovačič, L., Becker, S., Boelens, R. and Griesinger, G. (2011): Cys-Ph-TAHA: A lanthanide binding tag for RDC and PCS enhanced protein NMR. *J. Biomol. NMR* 51, 329–337.

### Organization of conferences, congress and meetings

1. 6th FP EC, "9th CONCO Meeting", Brdo, Slovenia, 26-27 January 2011

# INTERNATIONAL PROJECTS

- Applied Venomics of the Cone Snail Species *Conus consors* for the Accelerated, Cheaper, Safer and More Ethical Production of Innovative Biomedical Drugs CONCO 6. FP EC, Integrated Project
  - 037592, LSHB-CT-2007-03792

EC; Dr. Reto Stöcklin, Atherís Laboratories, Plan-les-Quates, Geneva, Switzerland Prof. Igor Križaj

2. A Genome-scale Approach to Maximization of Triacylglycerol Biosynthesis in Yeast BI-AT/11-12-014

Dr. Klaus Natter, University of Graz, Institute of Molecular Biosciences, Graz, Austria Prof. Igor Križaj

3. 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 BI-BG/11-12-006

Dr. Svetla Petrova-Chankova, Sofia University "St. Kliment Ohridski", Sofia, Bulgaria Prof. Igor Križaj

 Isolation of Long-Nosed Viper (Vipera ammodytes ammodytes) Venom Components and Analysis of their Immunogenicity BI-HR/10-11-025

Dr. Beata Halassy, Imunološki zavod, d.d., Odjel za istraživanje i razvoj, Zagreb, Croatia Prof. Igor Križaj

 Changes in Spatiotemporal Dynamics of Endocytosis Upon membrane Pertubation BI-US/11-12-002

Dr. David Drubin, Department of Molecular and Cell Biology, University of California, Barkeley, CA, USA

# R & D GRANTS AND CONTRACTS

- 1. Photostability of selected industrial chemicals and their influence on the environment Asst. Prof. Uroš Petrovič
- Regulatory genomics: origin and evolution of the complex transcriptional regulatory network in vertebrates Asst. Prof. Dušan Kordiš
- Apoptotic effects of alkylpyridinium compounds on lung adenocarcinoma cells Prof. Igor Križaj
- Molecular description of lipid membrane changes in disease Prof. Igor Križaj
- 5. Data and knowledge integration methods for network systems biology Asst. Prof. Uroš Petrovič
- The role of secretory phospholipases A2 in breast cancer Prof. Jože Pungerčar
- Proteins of the long-nosed viper venom acting on haemostasis development of innovative biomedical antithrombotics Prof. Igor Križaj
- 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
- 10. Antiretroviral APOBEC3 proteins and their role in retroelement defense Prof. Igor Križaj
- Knowledge technology approaches in drug discovery: analysis and experiment planning in high-throughput genetics Asst. Prof. Uroš Petrovič
- Structural explanation of the high increase in enzymatic activity of secreted phospholipases A2 in complex with calmodulin by high resolution NMR Dr. Lidija Kovačič

## RESEARCH PROGRAM

 Toxins and biomembranes Prof. Igor Križaj

### MENTORING

### Ph. D. Thesis

 Katja Škerget, Contribution to understanding of the mechanism of amyloid fibril formation and its effects on the cell (mentor Eva Žerovnik; co-mentor Uroš Petrovič).

### VISITORS FROM ABROAD

Postgraduates

10. Vesna Brglez, B. Sc

11. Minca Ferlin, B. Sc.

12. Borut Jerman, B. Sc.

13. Petra Kaferle, B. Sc.

Janez Kokošar, B. Sc.
 Jernej Oberčkal, B. Sc.

17. Tamara Sajevic, B. Sc.

Technical and administrative staff

16. Anja Pucer, B. Sc.

Igor Koprivec
 Darja Žunič Kotar

- Berta Avila Gratacos, University of Barcelona, Faculty of Pharmacy, Spain, 27 September 2010 – 31 March 2011
- Dr. Kristina Radošević, Faculty of Food Technology, University of Zagreb, Croatia, 4 April – 4 July 2011
- Dr. Alenka Čopič, Department of Biological Sciences, University of Columbia, USA, 30 September 2011
- Dr. Marija Brgles, Dr. Beata Halassy, M. Sc. Maja Lang Balija, B. Sc. Tihana Kurtović, Institute of Immunology, Zagreb, Croatia, 24 October 2011
- Dr. Vasili Atanasov, Department of Analytical Chemistry, Sofia University "St. Kliment Ohridski", Sofia, Bulgaria, 4–23 December 2011

### STAFF

#### Researchers

- 1. Asst. Prof. Dušan Kordiš
- 2. Prof. Igor Križaj, Head 3. Asst. Prof. Uroš Petrovič
- 4. Prof. Jože Pungerčar
- Postdoctorial associates
- 5. Dr. Lidija Kovačič
- 6. Dr. Adrijana Leonardi
- 7. Dr. Mojća Mattiazzi Ušaj
- 8. Asst. Prof. Toni Petan
- 9. Dr. Jernej Šribar

# BIBLIOGRAPHY

### **ORIGINAL ARTICLES**

- Beata Halassy, Marija Brgles, Lidija Habjanec, Maja Lang Balija, Tihana Kurtović, Martina Marchetti Deschmann, Igor Križaj, Günter Allmaier, "Intraspecies variability in Vipera ammodytes ammodytes venom related to its toxicity and immunogenic potential", *Comp. biochem. physiol., Toxicol. pharmacol.*, vol. 153, no. 2, pp. 223-230, 2011.
- 2. Silke Kauferstein, Christine Porth, Yvonne Kendel, Annette Nicke, Dušan Kordiš, Philippe Favreau, Reto Stöcklin, Dietrich Mebs, "Venomic study on cone snails (Conus spp.) from South-Africa", *Toxicon (Oxford)*, vol. 57, issue 1, pp. 28-34, 2011.
- 3. Dušan Kordiš, "Extensive intron gain in the ancestor of placental mammals", *Biology direct*, vol. 6, article no. 59, 8 pp., 2011.
- 4. Tihana Kurtović, Marija Brgles, Adrijana Leonardi, Maja Lang Balija, Igor Križaj, Günter Allmaier, Martina Marchetti-Deschmann, Beata Halassy, "Ammodytagin, a heterodimeric metalloproteinase from Vipera ammodytes ammodytesvenom with strong hemorrhagic activity", *Toxicon (Oxford)*, vol. 58, issue 6-7, pp. 570-582, 2011.
- Karim Malki et al. (21 authors), "Convergent animal and human evidence suggests a role of PPM1A gene in responseto antidepressants", *Biol. psychiatry* (1969), vol. 69, issue 4, pp. 360-365, 2011.
- Dietrich Mebs, Dušan Kordiš, Yvonne Kendel, Silke Kauferstein, "The evolution of *αD*-conopeptides targeting neuronal nicotinic acetylcholine receptors", *Acta chim. slov.*, vol. 58, no. 4, pp. 730-734, 2011.
- 7. Fabian Peters, Mitcheell Maestre-Martinez, Andrei Leonov, Lidija Kovačič, Stefan Becker, Rolf Boelens, Christian Griesinger, "Cys-Ph-TAHA: a lanthanide binding tag for RDC and PCS enhanced protein NMR", *J. Biomol. NMR*, vol. 51, no. 3, pp. 329-337, 2011.

- 8. Jure Pohleven, Jože Brzin, Lara Vrabec, Adrijana Leonardi, Andrej Čokl, Borut Štrukelj, Janko Kos, Jerica Sabotič, "Basidiomycete Clitocybe nebularis is rich in lectins with insecticidal activities", *Appl. microbiol. biotechnol.*, vol. 91, no. 4, pp. 1141-1148, 2011.
- 9. Blanka Premrov Bajuk, Irena Zdovc, Vida Smrekar, Igor Križaj, Adrijana Leonardi, Marinka Drobnič-Košorok, "Dermatophyte Trichophyton mentagrophytes produces cysteine protease inhibitor", *Acta chim. slov.*, vol. 58, no. 1, pp. 33-40, 2011.
- Tamara Sajevic, Jurij Reščič, Vojko Vlachy, "Correlation between flexibility of chain-like polyelectrolyte and thermodynamic properties of its solution", *Condens. matter phys.*, vol. 14, no. 3, art. no. 33603 (14 pp.), 2011.

### **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

- Dušan Kordiš, "Evolution of Phospholipase A[sub]2 toxins in venomous animals", Acta chim. slov., vol. 58, no. 4, pp. 638-646, 2011.
- Igor Križaj, "Ammodytoxin: a window into understanding presynaptic toxicity of secreted phospholipases A<sub>2</sub> and more", *Toxicon (Oxford)*, vol. 58, issue 3, pp. 219-229, 2011.
- 3. Jože Pungerčar, Petra Prijatelj, Toni Petan, "Structure-function relationship studies of ammodytoxins and ammodytins by protein engineering", *Acta chim. slov.*, vol. 58, no. 4, pp. 660-670, 2011.
- Tamara Sajevic, Adrijana Leonardi, Igor Križaj, "Haemostatically active proteins in snake venoms", *Toxicon (Oxford)*, vol. 57, no. 5, pp. 627-645, 2011.
- 5. Jernej Šribar, Igor Križaj, "Secreted phospholipases  $A_2$  not just enzymes", *Acta chim. slov.*, vol. 58, no. 4, pp. 678-688, 2011.

# 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.

During 2011 the research on fungal protease inhibitors involved the functional analysis of mycocypins and cospin as effectors of a fungal defence against predators, parasites and pathogens. The model organisms homobasidiomycete Coprinopsis cinerea and nematode Caenorhabditis elegans were used in collaboration with the group of Dr Markus Künzler in the laboratory of Prof Markus Aebi at the Institute of Microbiology of the Swiss Federal Head: Institute of Technology Zürich (ETH Zürich). We have determined that mycocypins are not nematotoxic, except Prof. Janko Kos under certain conditions, where the nematodes were under some other stress. In addition, an antinutritional effect was observed for some macrocypins, where nematodes fed with the inhibitors of digestive proteases (mycocypins) consumed all the available food, presumably due to ineffective nutrition exploitation, while control nematodes consumed approximately half of the available food. In order to address this issue in an ecologically more relevant model we prepared constructs for the heterologous expression of mycocypins (and a few other fungal proteins) in the model filamentous fungi Ashbya gossypii, which will be used in toxicity tests with the fungivorous nematode Aphelenchus avenae.



The characterization of the serine protease inhibitor cospin from the inky cap mushroom (Coprinopsis cinerea) that specifically inhibits trypsin was concluded. The genetic, biochemical and structural characterization was the result of a collaboration of three groups. The genetic and functional characterization was performed at ETH Zürich, the biochemical characterization was performed at the Department of Biotechnology (B3)

and the crystal structure was determined at the Department of Biochemistry and Molecular and Structural Biology (B1). The results were published in the Journal of Biological Chemistry, as cospin is the first trypsin inhibitor from mushrooms with a determined three-dimensional structure.

In the field of glycobiology, we continued studying lectins, a diverse group of carbohydrate-binding proteins, and their biological activity. 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 (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 biological activity of the lectins was examined on various systems. CNL showed the inhibition of the growth of human leukemic T lymphocytes (Jurkat cells) and the activation of human dendritic cells in a way to direct the Th1 immune response, which was also shown by CnSucL lectin. The immunomodulatory properties of these lectins could be potentially used in biomedicine concerning immune response-related diseases, to strengthen anti-tumour immune responses, or could be used for targeting specific

a fungal inhibitor of serine proteases, was determined.

The structure and biological role of cospin,



Figure 1: Testing of the nematotoxic action of inhibitors microcipins in nematode Caenorhabditis elegans

cells. Moreover, CnSucL exhibited toxicity against the fruit fly (Drosophila melanogaster), while CNL showed, in addition to D. melanogaster, toxicity against the insects Colorado potato beetle (Leptinotarsa decemlineata) and the mosquito Aedes aegypti, as well as the amoebozoa Acanthamoeba castellanii, and a hypersensitive



Figure 2: A: Structures of full-length cystatin F (pink) and cathepsin L (blue) B: Structures of full-length cystatin F (pink) and cathepsin S (purple). Magister, S., in sod., Eur. J. Cell Biol.

strain of nematode *Caenorhabditis elegans*. These results lead to the application of lectins in biotechnology as environmentally friendly agents for the control of crop pests.

The glycan microarray analysis revealed that the lectin is specific for a unique glycan, N,N'-diacetyllactosediamine (GalNAc $\beta$ 1–4GlcNAc, LacdiNAc), which is rare in mammals, but was found in tumour and leukemic cells and is abundant in invertebrates. Therefore, we hypothesize that the glycan represents the target for CNL to exhibit the effects. The three-dimensional structure of CNL in complex with LacdiNAc was determined and interactions between the lectin and the glycan were studied. Homodimeric CNL has two glycan-binding sites. CNL mutants that do not contain an active glycan-binding site or contain only one binding site were constructed and their activity examined on leukemic Jurkat cells and nematode C. elegans. The mutants were inactive, thus we have shown the glycan-binding property of CNL is essential for its activity and moreover, both binding sites are required.

An important part of our research in 2011 was focused on the role of proteases and protease inhibitors in malignant, immune and neurodegenerative processes. We studied the factors that regulate the differentiation of dendritic cells and their role in the activation of the T cell immune response. In dendritic cells we continued the studies on the role of a the cell maturation. Using immunofluorescence and electron microscopy.

endogenous protease inhibitors during the cell maturation. Using immunofluorescence and electron microscopy, we determined subcellular localization of cystatin F in immature, maturing adherent and mature DCs and its co-

Position-dependent splicing regulation by TDP-43 and its RNA targets has been characterised.



Figure 3: The interaction between lectin CNL in glycan N,N'diacetyllactosediamine (GalNAcβ1-4GlcNAc, LacdiNAc), Pohleven et al. (2011) J. Biol. Chem.

**y TDPcrised.** localization with cathepsins. In immature DCs cystatin F co-localizes with cathepsin S, after induction of DC maturation, however, it is translocated into lysosomes and co-localizes with cathepsin L. Besides co-localization studies we performed the enzyme kinetics of an N-terminally truncated hepsins S, H, L and X and modelling of the complexes between full-length cystatin F and

form of cystatin F with cathepsins S, H, L and X and modelling of the complexes between full-length cystatin F and cathepsins S and L. We showed that the N-terminally truncated form of cystatin F was a 12-fold-weaker inhibitor of cathepsin S than the full-length form, whereas no significant difference in inhibition was observed for cathepsins

L, H and X. The model of the interaction of full-length cystatin F with cathepsins S and L showed no significant difference in the binding of the cystatin F N-terminal region.

Based on our results we have concluded that cystatin F could regulate the activity of cathepsin L in maturing, adherent DCs and thus control the adhesion of DCs. On the other hand, the role of cystatin F in regulating cathepsin S activity and its function in Ii processing is still uncertain due to the weak binding of the truncated cystatin F, which is prevails intracellularly.

A DNA and RNA-binding protein Tar DNA-binding protein 43 (TDP-43) is involved in neurodegeneration processes in some neurological diseases, such as amyotrophic lateral sclerosis (ALS), frontotemporal lobar degeneration (FTLD), Alzheimer's disease and others. The protein is involved in the regulation of mRNA splicing and stability, miRNA biogenesis and acts as a transcriptional repressor. In disease, insoluble aggregates of TDP-43 form in neurons. We are investigating TDP-43 in cooperation with the Institute of Psychiatry, King's College London in the United Kingdom.

Last year, our research focused on the influence of TDP-43 on the expression of other cell proteins. We silenced and overexpressed TDP-43 in cells, respectively, and analysed and compared protein levels by mass spectrometry and immunodetection. The results show that TDP-43 regulates several RNAbinding proteins including FUS, another ALS and FTLD associated protein. Also, TDP-43 regulates RanBP1, which has an important role in cell cycle progression and nuclear transport.

An insight into the regulation of the expression of TDP-43 and in the extent of proteins regulated by TDP-43 will contribute to understanding its normal physiological function as well as enlighten its role in disease development and progression, the mechanisms of which are still unknown.

In the field of the research of lactic acid bacteria we continued with the optimization of the surface display on *Lactococcus lactis* with the help of the BmpA protein. We have prepared 18 genetic constructs of shortened versions

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of the protein BmpA gene. We have introduced an intermediary spacer region in half of them. In our further work we will test the ability of the prepared constructs for the surface display of model protein B domain.

We have established an ELISA assay for the determination of the titre of antibodies against antigen VP1-2a of the hepatitis A virus in mouse serum. With the use of the assay we determined the antibody titre in the serum of mice, which were orally vaccinated with recombinant bacterium *Lactococcus lactis*, expressing the hepatitis A virus antigen. We observed an increase in immune response following successive vaccine doses. Approximately half of

the mice in the group responded to oral vaccination. However, the response was, according to expectations, lower in comparison to the control group, which was parenterally administered with purified antigen.

We have also described the preparation of the TA-cloning system on the basis of the lactococcal vector pNZ8148, which enables the immediate ligation of

# The role of the proteins PGE2 and COX2 in the differentiation of dendritic cells was demonstrated.

Taq polymerase-amplified DNA with added 3'-adenosines. The plasmid pNZ-T was prepared with whole-plasmid PCR amplification with high fidelity and processivity DNA polymerase, which was followed by XcmI restrictions digest, yielding T-overhangs. The advantage of our approach is a high percentage of colonies with insert containing plasmid (above 95 %). This is due to the use of a linear PCR product, instead of a circular plasmid, for the XcmI digestion, which decreases the background of empty, non-digested plasmid. Additionally, our approach is flexible, since the position of the TA-cloning site is easily determined with the appropriate primer design. The approach is universal and can be applied to other plasmids and species.

Our research on the response of plants to water stress has involved a study of the crop plant Phaseolus vulgaris

and the model plant Ramonda sp., which is able to survive complete desiccation of their vegetative tissue. This collaboration is ongoing with the Agricultural Institute of Slovenia. In the previous year we identified and characterized three serine endopeptidases and five serine aminopeptidases in the leaves of a common bean variety, which are moderately sensitive to drought. With regards to desiccation-tolerant plants, following our previous studies on *R. serbica*, we have focussed attention on the related plant *R. nathaliae*. An analysis of the protein profile showed that protein expression

Candidate carrier proteins for surface display on *Lactococcus lactis* have been selected by theoretical and experimental analyses of the surface proteome - 31 scientific papers in journals with an impact factor were published in 2011

in the leaves of desiccated plants significantly differs from that in the watered plants.

The results of the research work at the Department of Biotechnology in 2011 were published in 31 scientific papers in journals with an impact factor, in four chapters in books and presented in scientific conferences as lectures and posters. The members of the department were very active also in pedagogical work, as lecturers and mentors to students preparing diploma and doctoral thesis at the University of Ljubljana, the University of Maribor and the Jožef Stefan Postgraduate School.

### Some outstanding publications in the last year

- Sabotič, Jerica, Bleuler-Martinez, Silvia, Renko, Miha, Avanzo Caglič, Petra, Kallert, Sandra, Štrukelj, Borut, Turk, Dušan, Aebi, Markus, Kos, Janko, Künzler, Markus. Structural basis of trypsin inhibition and entomotoxicity of cospin, a serine protease inhibitor involved in defence of Coprinopsis cinerea fruiting bodies. J Biol Chem, [in press] 2011.
- Tollervey, James R., Curk, Tomaž, Rogelj, Boris, Briese, Michael, Cereda, Matteo, Kayikci, Melis, König, Julian, Hortobágyi, Tibor, Nishimura, Agnes L., Župunski, Vera, Patani, Rickie, Chandran, Siddharthan, Rot, Gregor, Zupan, Blaž, Shaw, Christopher E., Ule, Jernej. Characterizing the RNA targets and position - dependent splicing regulation by TDP-43. Nat Neurosci, 2011, vol. 14, no. 4, 452-459
- Obermajer, Nataša, Muthuswamy, Ravikumar, Lesnock, Jamie, Edwards, Robert P., Kalinski, Pawel. Positive feedback between PGE2 and COX2 redirects the differentiation of human dendritic cells towards stable myeloidderived suppressor cells. Blood, 2011, vol. 118, no. 20, 5498-5505.

### Patent granted

 The use of glycosidases and glycosiltransferases for increased production of proteins David Dobnik, Špela Baebler, Jana Žel, Kristina Gruden, Dejan Štebih SI23374 (A), Urad RS za intelektualno lastnino, 30.11.2011.

### Awards and appointments

- 1. Sara Žigon was awarded for the graduation thesis.
- 2. Dr. Jerica Sabotič, Sara Žigon: Faculty Prešeren Award to the students of the Faculty of Pharmacy, the University of Ljubljana for 2011

### Organization of conferences, congress and meetings

1. Organization of the annual meeting of co-workers of the research program "Pharmaceutical biotechnology: knowledge for health" from the Department of Biotechnology at the Jozef Stefan Institute and the Chair of Pharmaceutical Biology at the Faculty of Pharmacy of the University of Ljubljana, Slovenia, 10 November 2011

## INTERNATIONAL PROJECT

 Bioactive Substances in Endemo-Relict Plants of the Balkan Peninsula BI-SR/10-11-014
 Dr. Branka Stevanović, University of Belgrade, Faculty of Biology, Belgrade, Serbia Prof. Janko Kos

## **R & D GRANTS AND CONTRACTS**

- 1. Expression and functional analysis of non-coding RNA in Parkinson disease
- Dr. Boris Rogelj
  Transport and RNA binding of TDP-43 and FUS implications for ALS/FTLD spectrum of neurodegenerative disease
- Dr. Boris Rogelj 3. Functional analysis of proteins resistant to drought and insects Dr. Jerica Sabotič
- 4. Inhibitors of cysteine carboxypeptidases as regulators of autoimmune and

# MENTORING

### Ph. D. Theses

- Petra Avanzo Caglič, Biochemical and biological properties of cnispin, a new serine protease inhibitor from muschroom Clitocybe nebularis (mentor Borut Štrukelj; comentor dr. Jerica Sabotič).
- Alenka Kužnik, The mechanism activation and inhibition of endosomal Toll-like receptors (mentor Roman Jerala; co-mentor Janko Kos).
- Bojana Mirković, Regulation of exopeptidase and endopeptidase activity of cathepsin B (mentor Janko Kos).
- Petra Nikolić, Gene expression patterns in grapevine leafs infected with phytoplasma associated with bois noir disease (mentor Marina Dermastia; co-mentor Kristina Gruden).
- Matjaž Ravnikar, Research of recombinant probiotics and interactions between probiotic lactic acid bacteria and drugs (mentor Borut Štrukelj; co-mentor Mojca Lunder).

### STAFF

#### Researchers

- 1. Prof. Kristina Gruden\*
- 2. Prof. Janko Kos\*, Head
- Dr. Boris Rogelj
   Prof. Borut Štrukelj\*
- Postdoctorial associates
- 5. Dr. Aleš Berlec
- Asst. Prof. Nataša Obermajer
- 7. Dr. Jure Pohleven
- 8. Dr. Jerica Sabotič

# BIBLIOGRAPHY

### ORIGINAL ARTICLES

 Safa Al-Sarraj, Andrew King, Claire Troakes, Bradley Smith, Satomi Maekawa, Istvan Bodi, Boris Rogelj, Ammar Al-Chalabi, Tibor Hortobágyi, Christopher E. Shaw, "p62 positive, TDP-43 negative, neuronal cytoplasmic and intranuclear inclusions in the cerebellum neurodegenerative processes Prof. Janko Kos

- Response to water stress in common bean (Phaseolus vulgaris L.): proteomic analysis and QTL mapping Prof. Janko Kos
- New biotechnological drugs obtained by phage display
- Prof. Borut Štrukelj
  Regulation of T-cell functions with alpha type 1-polarised (alphaDC1) and standard dendritic cells (sDC).
  Asst. Prof. Nataša Obermajer

### RESEARCH PROGRAM

- 1. Pharmaceutical biotechnology: Knowledge for health Prof. Janko Kos
- Ana Rotter, Development and implementation of system biology tools: a case study of plant physiology data analysis (mentor Andrej Blejec; co-mentor Kristina Gruden).
- Mehdi M. Saghafi, Donepezil and galantamin as a preventive protection against intoxocation with diizopropilfluorofosfat inhibitor of the enzyme AChE (mentor Fajko Bajrović; co-mentor Borut Štrukelj).

### M. Sc. Thesis

- 1. Milen Tewolde, Functional characterisation of TDP-43 in relevance to ALS (mentor Boris Rogelj; co-mentor Jacqueline Mitchell).
- 2. Neža Turnšek, Molecular basis of colorado potato beetle (Leptinotarsa decemlineata) response to plant defense response (mentor Kristina Gruden).

# VISITORS FROM ABROAD

- 1. Dr. Tamara Rakić, Biological Faculty, University of Belgrade, Belgrade, Serbia, 22–29 November 2011
- Dr. Marko Saboljević, Biological Faculty, University of Belgrade, Belgrade, Serbia, 2–8 December 2011

### Postgraduates

- 9. Dr. Petra Avanzo Caglič, left 01.05.11
- 10. Špela Magister, B. Sc.
- Maja Štalekar, B. Sc.
   Simon Žurga, B. Sc.

Technical and administrative staff

13. Darja Žunič Kotar

Note: \* part-time JSI member

and hippocampus define the pathology of C9orf72-linked FTLD and MND/ALS", *Acta Neuropathol*, vol. 122, no. 6, pp. 691-702, 2011.

2. Špela Baebler, Katja Stare, Maja Kovač, Andrej Blejec, Nina Prezelj, Tjaša Stare, Polona Kogovšek, Maruša Pompe Novak, S. Rosahl, Maja Ravnikar, Kristina Gruden, "Dynamics of responses in compatible potato - potato virus Y interaction are modulated by salicylic acid", *PLoS one*, vol. 6, issue 12, pp. 1-12, 2011. 3. Aleš Berlec, Petra Zadravec, Zala Jevnikar, Borut Štrukelj, "Identification of candidate carrier proteins for surface display on Lactococcus lactis by theoretical and experimental analyses of the surface proteome", *Appl. environ. microbiol.*, vol. 77, no. 4, pp. 1292-1300, 2011.

- 4. Silvia Bleuler-Martinez, A. Butschi, M. Garbani, M. A. Wälti, T. Wohlschlager, E. Potthoff, Jerica Sabotič, Jure Pohleven, P. Lüthy, M. O. Hengartner, Markus Aebi, Markus Künzler, "A lectin-mediated resistance of higher fungi against predators and parasites", *Mol. ecol.*, vol. 20, no. 14, pp. 3056-3070, 2011.
- Ivanka Cizelj, Rebeka Lucijana Berčič, Daliborka Dušanić, Mojca Narat, Janko Kos, Peter Dovč, Dušan Benčina, "Mycoplasma gallisepticum and Mycoplasma synoviae express a cysteine protease CysP, which can cleave chicken IgG into Fab and Fc", *Microbiol (Soc. Gen. Microbiol.)*, vol. 157, no. 2, pp. 362-372, 2011.
- 6. Jeff D. Colbert, Stephen P. Matthews, Janko Kos, Colin Watts, "Internalization of exogenous cystatin F supresses cysteine proteases and induces the accumulation of single-chain cathepsin L by multiple mechanisms", *J Biol Chem*, vol. 286, no. 49, pp. 42082-42090, 2011.
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# DEPARTMENT OF ENVIRONMENTAL SCIENCES **()**-2

The basic characteristic of the Department of Environmental Sciences is multidisciplinarity, as our researches comprehend different fields in natural and social sciences, especially physical, chemical, geological and biological processes that affect our environment, society and human activities. Above all, we wish to explain the connections between natural processes and human activities, and the influences of these activities on human and environmental health. We combine scientific excellence of research work with solving concrete technological problems in industry, education and development, covered by the research fields of analytical chemistry, radiochemistry and radioecology, biological and geochemical cycles of elements, nutrition and health of humans, animals and plants, waste management, mathematical and GIS modelling of environmental processes, and risk and environmental impact assessment.

### **Environmental analytical chemistry**

A new analytical method was developed for the speciation of methy- butyl-, phenyl- and octyltin compounds Head: in landfill leachates. The optimal pH of ethylation was adjusted by citrate buffer, while ethylated organotin com- Prof. Milena Horvat pounds were extracted into hexane and their quantitative determination was performed by gas chromatography coupled to ICP-MS.

By the use of the high matrix introduction system (HMI) and high energy collision mode (HECM) applying high He flow rates into a collision cell, the ICP parameters were optimised enabling an efficient introduction of samples with high salt content and a reduction of polyatomic interferences of chlorine and carbon ions in the determination of chromium at masses 52 and 53. In this investigation, stable chromium isotopes (<sup>51</sup>Cr and <sup>53</sup>Cr) were used. The optimised detection procedure was successfully applied in the chromium speciation analysis by FPLC-ICP-MS.

In the field of research for cancer therapy, an analytical procedure was developed for determining the distribution of Pt-based chemotherapeuticals in the serum of cancer patients by using the convective-interaction media (CIM DEAE-1) column coupled to inductively coupled plasma mass spectrometry (ICP-MS). It was experimentally proven that the use of the monolithic column was complementary to the particle-packed Mono Q FPLC column and that the separation on the CIM DEAE-1 column is faster and more robust. By the use of the CIM column, more than 150 successive serum separations can be performed without applying a cleaning procedure, while only 6 can be performed if the FPLC column is used.

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 antiinflammatory drugs, lipid regulators and hormones investigated in the past, we introduced a series of analytical procedures to enable a determination of new compounds like cytostatics, tranquilisers, antidepressants and endocrine disrupting compounds (bisphenol A, triclosan, benzophenones, etc.) in various matrices such as surface and waste water as well as biological samples.

In the area of steroid estrogens we have introduced a modified estrogenicity assay (NE-ER Calux), a fast and user-friendly way of determining the estrogenicity of the environmental samples. We compared applicability of this assay with the previously validated estrogenicity tests (the standard ER-Calux as well as the estrogenicity based on the GC-MSD calculation) on the "real" waste-water samples. The results showed great applicability of NE-ER Calux, as the time consuming and expensive sample extraction is thus avoided allowing a large number of samples to be analysed. In the area of industrial endocrine disrupting compounds, analytical methods for determining bisphenol A, triclosan, parabens and various benzophenones in urine were developed and will be applied to a large-scale monitoring within the EU 7FP DEMOCOPHES project.

For the purpose of food quality and safety control in the Slovenian market, the isotope methods for authentication (geographic origin) and

- A model was built to forecast the radon concentration in the Postojna Cave on the basis of the difference between the outside and the cave-air temperatures; a time delay of about 3 to 4 days occurs between the change in the outside temperature and the change in radon concentration.
- The assessed combined annual effective ingestion dose due to 210Po and 210Pb for fish, squid and mussels consumed in Slovenia is 47.6 µSv.
- In the area of organic analytical chemistry we developed new methods for determining the trace levels of pharmaceuticals and their products in the environmental matrices.
- An international meeting on metrology issues related to mercury measurements in the marine environment set up the basis for a global observation strategy to assure comparability of the measurement results.

**Outstanding achievements:** 



detection of the frauds in milk and dairy products were optimized and validated. The methods for the isolation and the compound-specific analysis of the stable isotope composition of C and N in milk proteins (in particular casein) were optimized and validated.

In 2011 the  $k_0$ -INAA has also been improved. We re-measured the neutron flux in typical irradiation channels of the TRIGA reactor and validated the MATSSF software (developed at the JSI) for calculating the self-shielding factors (thermal and epithermal). We participated in the re-evaluation of  $Q_0$  for Rh-103 and the  $k_0$  factors for Rh-104 needed for updating the KAYZERO library, that are validated by adding a mass of certified standard solution of Rh to cellulose pellets.

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-DB001 *Human hair* (As, Cd, Cu, Hg, Pb, Se and Zn), (ii) ERM-CD200 *Fucus vesiculosus* (As, Cd, Hg, Se and Zn) and (iii) ERM-CE278k *Mussel tissue* (Ag, As, Cd, Cr, Cu, Fe, Hg, Mn, Ni, Pb, Rb, Se, Sr and Zn). 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 2012, which will later be entered in the KCDB (*Key Comparisons Data Base*).

#### **Biological and geochemical cycles**

Stable isotopes of carbon were used in the studies of carbon cycling and carbon balance in different natural environments. Contributions of dolomite and calcite weathering of bedded carbonate bedrock in the Sava and Soča catchments to the overall carbon balances of the streams were evaluated. The contribution of carbonate weathering to the  $CO_2$  balance in soil atmosphere in different types of forests and grassland at Podgorski Kras was quantified. Isotope analyses of coal-bed gases occurring in the Velenje coal seams revealed that  $CO_2$  is likely to be sourced from a mixture of an in-situ microbial activity and the external  $CO_2$ , while  $CH_4$  is predominantly sourced from microbial methanogenesis, with a possible addition of the thermogenic gas from deeper formations, and an influence of microbial oxidation of methane. For the first time in Slovenia, a systematic investigation of environmental



Figure 1: Longitudinal cross-section of the Postojna Cave; indicated are the directions of air movement (with radioactive and non-radioactive aerosols) in the summer and winter (pink arrows – warmer air, blue arrows – colder air) and our measurement points for the continuous radon monitoring (Great Mountain, Beautiful Caves, The Lowest Point). The air movement is controlled mainly by the outside temperature which, as a consequence, strongly influences the radon concentration in the cave air, being 2-3 times higher in the summer than in the winter: (Cave cross-section adopted after Gospodarič, 1976).

isotopes in snow hydrology was started in collaboration with Lomonosow State University in Moscow.

For the vulnerability assessment and identification of suitable remediation measures in the degraded Idrija Hg-mine ecosystem, a spatial distribution of Hg in soils and atmosphere was assessed, the magnitude of atmospheric deposition determined, and the Hg emission and erosion models developed within the GIS environment. Spatially designed approach will serve as a basis for selecting the suitable cost-effective remediation technologies and scenarios design.

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 collaboration with the GMOS consortium and GEOTRACESRS network, a workshop entitled *Mercury in the Marine Environment: a global metrology challenge* was organized between 9 and 12 May 2012 in Piran. Over 60 well known experts from all over the world were present. In November 2011, the first Mediterranean cruise was organized for the Western Mediterranean on a research vessel Urania.

Studies concerned with the transfer of natural radionuclides in the ecosystems with enhanced levels of natural radioactivity like the former uranium mine and mill at Žirovski vrh, and in several areas of Central Asia, were carried out. Fractionation of the natural radionuclides in the soil as well as their transfer into the ecosystem and food chain were studied. The transfer of radionuclides from the uranium-radium decay chain into plants and milk

was assessed. Environmental radiological risks were assessed using the ERICA Tool. At the same time, measurement procedures for determining alpha emitters, particularly <sup>226</sup>Ra in water, were upgraded.

In 2011 we continued to investigate the distribution of <sup>129</sup>I in samples of sea water, algae, mussels and sediment from the Bay of Trieste and Piran. The <sup>129</sup>I/<sup>127</sup>I isotopic ratios observed were in the range from 0.8 to 3.0 E-08 for seawater, from 0.06 to 0.35 E-08 for marine sediment, from 0.05 to 0.10 E-08 for the brown alga *Fucus virsoides* and from 0.3 to 0.9 E-08 for the Mediterranean mussel *Mytilus galloprovincialis*. These are the first results obtained for the North Adriatic and Mediterranean Sea.

In the framework of the bilateral cooperation between Slovenia and Brazil (BI-BR/10-12-002), we continued with the characterization of arsenic in contaminated sites.

Radon research has been focused on (i) a study of geophysical processes of radon transport in the karst caves and in soil gas and (ii) the relationship between the concentration of the radioactive nano aerosols of radon progeny and the size distribution of the general, non-radioactive aerosols. In the karst caves (Postojna and Kostanjevica) the influence of hydro-meteorological changes in the outdoor environment and in the caves on radon concentration in the caves has been studied. The difference between the outside and the cave air temperatures is crucial in controlling the radon levels. The time delay between the changes in the outside air temperature and the changes in the radon level in the cave has been studied. We also continued the research on the affect of seismic activity and tectonic faults on the radon levels, which is a part of the international project BlackSeaHazNet carried out within the 7FP. The transport of radon and carbon dioxide, the radon carrier, has been studied in soil gas at different geological bedrocks in Slovenia and Japan (the Japanese-Slovene bilateral project). The aim of the combined study of the radioactive radon progeny aerosols and general aerosols in the size range from 10 to 1100 nm was to indicate the size distribution of general aerosols that affect most significantly the ratio of the attached-unattached radon progeny. The research was performed in the Postojna Cave with a low general-aerosol concentration and an elevated concentration of radon progeny, and in a dwelling with the usual concentration of general aerosols and a slightly increased concentration of radon progeny. In the second case the influence of various activities (cooking, candle burning, smoking), producing aerosol particles of different sizes and concentrations, on the change in the attached-unattached radon progeny ratio has been studied.

### Environment, nutrition, health

In the framework of the *Life*+ project DEMOCOPHES, which aims at testing the methodology for a cross-European human biomonitoring protocol, the sampling of the test population started in November 2011. The sampling was performed in two primary schools: Šmarje pri Jelšah and Ljubljana (Vodmat). In the pilot phase the exposure of the target population of children between 6 and 11 years and their parents will be assessed. The compounds investigated included cadmium, mercury, cotinin, creatinine and the endocrine disrupting chemicals: phthalates, bisphenol A – BPA, parabens and triclosans.

In the area of arsenic research the MT mRNA expression was studied in human glioblastoma cell line U87 MG (American Type Culture Collection, USA) before and after an arsenic trioxide exposure. Gene expression of six metallothionein (MT) (sub) isoforms, namely *MT2a*, *MT1* (*a*, *e*, *f*, *x*) and *MT3*, was followed by qPCR. Cells were treated by arsenic (0.6-7 $\mu$ M) up to 48h with or without a vitamin C addition. Suppressed expression was observed after an exposure to a low concentration (<1  $\mu$ M As) and increased expression after an exposure to higher concentrations, especially for isoforms *MT1* (*f*, *x*) and *MT2a*. Both phenomena were tested with cadmium and

mercury exposures (0.6-10  $\mu$ M and 0.6-2  $\mu$ M, respectively). Results are interesting with respect to chemoresistance during a cancer treatment and the resistance against toxic effects of metals present in food and water or in a working environment (occupational exposure). At the same time the uptake of arsenic in the presence of vitamin C was studied in the same cells and found to be significantly decreased. Vitamin C is commonly used as an adjuvant believed to be synergistic with the arsenic trioxide effects. However, the obtained results questioned this belief. Although the methylation of arsenic is typical for liver cells, we confirmed its presence in the human glioblastoma cells. Since most of such experiments are conducted in a cell-culture environment we first examined the stability of arsenite in relevant conditions and found that stability varies with the composition of media. An addition of vitamin C can cause a particularly fast unwanted oxidation of arsenite to arsenate.

In addition to the biomedical research we also studied arsenic in the marine environment and food. In the 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 is little data on arsenic speciation in the ray samples and other Cartilagineous fish and our study shows similarities in arsenic speciation with the 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 the desert plant *Atriplex atacamensis*, grown wild in arsenic-polluted arid areas of Chile.

The metabolism of metals is tightly interfering with the selenium metabolism. Found in different selenoproteins, in the form of selenocystein, selenium is a vital part of antioxidative mechanisms necessary for the cells' survival. We tried to identify biomarkers of the selenium status caused by an oxidative stress after a long-term intensive



physical activity of a group of soldiers. We found out that no biomarker is exceptional, as all of them (blood, serum, plasma selenoprotein P Se conc., plasma and erythrocytes GPx activity) represent the situation most appropriately.



Figure 3: International conference entitled "Mercury in the marine environment: a global metrology challenge" was organized in May in Piran in the Framework of the COST, GEOTRACES and EU project GMOS. The world's best experts and instrument producers in the area of Hg research in the marine environment attended the workshop.

Although Se has not been confirmed to be an essential micronutrient in higher plants, it is known that they are capable of accumulating higher amounts of the element. These plants can accumulate a high amount of Se; however, not the total Se content, but its species present, parallels the Se bioavailability. The data about the Se content in water plants is very scarce. We investigated the uptake of Se and its compounds in the water moss (*Fontinalis antipyretica*), because it is common in the streams and rivers in Slovenia and worldwide. It was found to contain up to 3mg/kg of dry mater. The fraction of insoluble Se compounds in the residue, after an enzymatic hydrolysis using Protease (XIV), was around 75%. Soluble Se compounds in the extract were separated and measured using HPLC coupled with ICP-MS and only Se(VI) and Se(IV) were found. No Se-amino acids were detected.

The potential of nitrogen stable isotopes as a marker to reveal the history of nitrogen fertilization of organically vs. conventionally grown lettuce was investigated. It was found that the split and combined usage of the fertilisers can be detected only when the difference in  $\delta$ 15N between the applied synthetic and organic nitrogen fertilisers is very large (> 9.1‰). The N isotope analyses of different sorts of vegetables in the Slovenian market showed that the N isotopes can be used as an additional, but not an exclusive method of fraud detection.

### **Environmental monitoring**

The national human biomonitoring programme continued in collaboration with the regional health institutes, the Clinical Center in Ljubljana and regional hospitals, in particular with the gynaecologists and nurses. The HBM is conducted under the supervision of the Slovenian Chemical Administration Agency. We study the exposure to toxic chemicals including toxic metals (Hg, Pb, Cd), other elements (Se, As, etc.), and the persistent organic contaminants (POPs) including dioxines, furans, pesticides, PCBs, brominated and fluorinated compounds. Human blood, urine, maternal milk and hair samples are collected for the analyses of the chemicals in question. The results will be used for establishing reference values and for assessing the exposure to toxic chemicals in Slovenia.

Regular programmes of monitoring isotopes in precipitation and rivers in Slovenia ( $\delta^{18}$ O and  $\delta^{2}$ H in rain, snow and surface waters of the Sava River) were continued. The data was also used for interpreting the atmospheric circulation patterns and atmospheric deposition of mercury in the Idrija basin. The department participated in the maintenance of the EU database on the isotopic composition of wine established in line with the EU regulation.

In collaboration with the Environmental Agency of the Republic of Slovenia the monitoring of organotin compounds in the surface and sea waters was continued in 2011.

An environmental-surveillance monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski Vrh was performed.

In the framework of the EU project Hydronet aiming at developing the robot systems for advanced water monitoring, tests were performed in the lagoons of Grado and Marano, in the coastal area of Livorno, and in Most na Soči.

#### Clean technologies and waste management

in the framework of the Slovenian-Chinese cooperation two workshops were organized: the first one was held on 17–19 September 2011 in Hangzhou, China, and the second one took place on 10–11 November 2011 in Ljubljana, Slovenia. The goal of the workshops was to foster the cooperation in research and education in the field of removing the pollutants from waste gases. An agreement was signed with the aim to join specific knowledge of the partners in order to respond more efficiently to the needs for the prevention of the pollution with gaseous emissions. This will be achieved through our cooperation in the scientific development, training of personnel and application of the knowledge developed.

The applicability of the electric arc furnace (EAF) black steel slag in asphalt mixes for road construction was critically evaluated. Long-term environmental impacts were assessed with the leachability tests based on the diffusion and speciation analyses. It has been experimentally proven that the investigated EAF slag can be considered as an environmentally safe substitute for natural aggregates in asphalt mixes.

With regard to the pharmaceutical residues, we focused on the elimination of selected pharmaceuticals in an optimised pilot waste-water-treatment plant, where the attention was given to the contaminant elimination mechanisms (biodegradation, photodegradation and adsorption as well as biomass adaptation), the application of different treatment technologies (ozonation, ClO<sub>2</sub>, UV and photocatalytic treatment, cavitation, biological (attached biomass) treatment, etc.) and the stable transformation product identification formed during the waste-water treatment and in the environment. We succeeded in identifying a number of pharmaceutical transformation products

and degradation pathways. Our research has also focused on the toxicity of the identified transformation products, and the results so far have shown that the transformation products can have a greater toxicity than the parent compounds.

### Risk and environmental impact assessment

The projects in 2011 were primarily associated with the strategic (spatial) environmental evaluation and the environmental & health assessment. Work on the project iNTeg-Risk requires an integration of a strategic, sustainability and project-level environmental evaluation with a spatial planning for the new emerging risk technologies. The environmental consultancy activities related to the construction of the NPP Krško 2 focuses on a comparative assessment involving nuclear and other options as a basis for deciding on the implementation of the project.

The radiological risk assessment of the organisms exposed to the influence of the former uranium mine and mill at Žirovski Vrh was evaluated by means of appropriate modelling tools. The ingestion dose to the general population due to marine-food consumption was also assessed.

### Some outstanding publications in the past year

- Gregorič Asta, Zidanšek Aleksander, Vaupotič Janja. Dependence of radon levels in the Postojna Cave on outdoor air temperature. Nat. Hazards Earth Syst. Sci., 11 (2011), 1523–1528.
- Kocman David, Vreča Polona, Fajon Vesna, Horvat Milena. Atmospheric distribution and deposition of mercury in the Idrija Hg mine region, Slovenia. Environ. Res., 2011, 111/1, 1-9.
- Kontić Branko, Kontić Davor. A viewpoint on the approval context of strategic environmental assessments. Environ. Impact. Asses. Rev., 2011, 32/1, 151-155.
- 4. Kosjek Tina, Heath Ester. Occurrence, fate and determination of cytostatic pharmaceuticals in the environment. TrAC, Trends Anal. Chem., 2011, vol. 30, issue 7, 1065-1087.
- Mechora Špela, Cuderman Petra, Stibilj Vekoslava, Germ Mateja. Distribution of Se and its species in Myriophyllum spicatum and Ceratophyllum demersum growing in water containing Se (VI). Chemosphere (Oxford), 2011, 84, 11, 1636-1641.
- Štrok Marko, Smodiš Borut. Levels of <sup>210</sup>Po and <sup>210</sup>Pb in fish and molluscs in Slovenia and the related dose assessment to the population. Chemosphere (Oxford), 2011, 82, 7, 970-976.
- Vahčič Mitja, Milačič Radmila, Ščančar Janez. Development of analytical procedure for the determination of methyltin, butyltin, phenyltin and octyltin compounds in landfill leachates by gas chromatography-inductively coupled plasma mass spectrometry. Anal. Chim. Acta, 2011, 694, 21-30.

### Awards and appointments

- 1. Asta Gregorič: »Outstanding Student Poster (OSP) Award» for »Radon concentration and ventilation in two different passages in the Postojna Cave», European Geoscience Union (EGU), General Assembly, Vienna, Austria, 3-8 April 2011
- Miha Avberšek: Best conference paper »Determination of steroid estrogens in waste waters without sample extraction«, 3rd Jožef Stefan International Postgraduate School Students Conference, 25 May 2011
- doc. dr. Radmila Milačič: Pregl Award for Exceptional Achievements for important scientific contributions in the field of speciation of elements, Ljubljana, Slovenia, 20 June 2011
- 4. dr. Tjaša Kanduč: Best Poster Award for »Mytilus galloprovincialis as a bioindicator of environmental conditions: the case of the eastern coast of the Adriatic Sea», European Society for Isotope Research, Isotope Workshop XI, Budapest, Hungary, 4-8 July 2011

### Organization of conferences, congress and meetings

- Janja Vaupotič: Training »Radon in buildings: measures to reduce its concentrations« SCOPES, Ljubljana, Slovenia, 5-6 May 2011; 10-11 November 2011
- 2. Milena Horvat, Nives Ogrinc: Workshop »Mercury in the marine environment: a global metrology challenge«, Piran, Slovenia, 9-12 May 2011
- 3. Milena Horvat: Workshop »Development of processes and equipment for flue gas purification«, Ljubljana, Slovenia, 9-11 November 2011
- Ljudmila Benedik: Training in radiochemistry and radioactivity measurements for practitioners from the countries eligible under the JRC Enlargement & Integration Policy, Ljubljana, Slovenia, 21 November to 2 December 2011



Figure 4: In the framework of the EU project GMOS – Global Mercury Observing System a research cruise FENICE was implemented in the Western Mediterranean to measure Hg distribution in the surface and depth profiles. The dissolved elemental mercury in water is a good proxy of the natural presence of this toxic metal in the Mediterranean waters.

# INTERNATIONAL PROJECTS

1. Complex Research of Earthquake's Prediction Possibilities, Seismicity and Climate Change Correlations BlackSeaHazNet 14. 7. FP. 246874 EC; Dr. Strachimir Mavridiev, Bulgarian Academy of Science, Institute of Nuclear Research and Nuclear Energy, Sofia, Bulgaria Prof. Janja Vaupotič 2 Fate and Effects of Cytostatic Pharmaceuticals in the Environment and the Identification of Biomarkers for and Improved Risk Assessment on Environmental Exposure CytoThreat 7. FP, 265264 EC; Nacionalni inštitut za biologijo, Ljubljana, Slovenia Prof. Ester Heath Global Mercury Observation System GMOS 7. FP, 265113 EC; Prof. Nicola Pirrone, CNR - Consiglio Nazionale delle Ricerche, Rome; Mario Gensini, CNR - Istituto sull'Inquinamento Atmosferico Sezione di Rende, c/o Polifunzionale UNICAL, Rende, Italy Prof. Milena Horvat 4. Coordinating Earth and Environmental Cross-Disciplinary Projects to promote GEOSS EGIDA 7. FP, 265124 EC; Pier Francesco Moretti, CNR, Consiglio Nazionale delle Ricerche, Department of Earth and Environment, Rome, Italy Asst. Prof. Sonia Loien European Coordinaton Action on Human Biomonitoring 5 COPHES 7. FP. 244237 18. EC; Dr. Alexandra Polcher, BiPRO GmbH, Beratungsgesellschaft für integrierte Problemlösungen, München, Germany Prof. Milena Horvat 6 Arctic Health Risks: Impacts on Health in the Arctic and Europe Owing to Climateinduced Changes in Contaminant Cycling ArcRisk 7. FP, 226534 EC; Arctic Monitoring and Assessment Programme, Secretariat, Oslo, Norway Prof. Milena Horvat 7. Floating Sensorised Networked Robots for Water Monitoring HYDRONET 7. FP, 212790, FP7-ENV-2007-1 EC; Dr. Monica Vignoni, Scuola Superiore di Studi Universitari e di Perfezionamento Sant'Anna, Pisa, Italy Prof. Milena Horvat Early Recognition, Monitoring and Integrated Management of Emerging, New 8. Technology Related Risks iNTeg-Risk 7. FP 213345, NMP2-LA-2008-213345 EC; European Virtual Institute for Integrated Risk Management, Stuttgart, Germany Prof. Branko Kontić, Asst. Prof. Marko Gerbec Mobilising Citizens for Vital Cities Ljubljana-Gent-Zagreb-Brno-Porto CIVITAS-ELAN 7. FP, 218954, TREN/FP7TR/218954 EC; Zdenka Šimonovič, Mestna občina Ljubljana, Ljubljana, Slovenia Dr. Davor Kontić, Prof. Branko Kontić, Asst. Prof. Marko Gerbec 10. Public Health Impact of Long-term, Low-level Mixed Element Exposure in Susceptible Population Strata PHIME 6. FP, 016253 EC; Ingela Byström, Prof. Staffan Skerfving, Lund University Hospital, Department of 24. Occupational and Environmental Health, Lund, Sweden Prof. Milena Horvat 11. DEMOCOPHES LIFE PLUS Programme LIFE 09 ENV/BE/00041 EC Prof. Milena Horvat 12. Access to Technology and Know-how in Cleaner Production in Central Europe ACT CLEAN

Central Europe Programme

EC; Jakob Gross, Horst Pohle, Federal Environment Agency, Dessau-Roßlau, Germany Asst. Prof. Sonja Lojen, Tanja Zdolšek, Andrej Gyergyek, B. Sc., Dr. Andrej Stergaršek

13. The Ocean Chemistry of Bioactive Trace Elements and Paleoclimate Proxies COST ES0801

- EC; COST Office, Brussels, Belgium Prof. Nives Ogrinc
  14. Stable Isotopes in Atmosphere-Biosphere-Earth System Research SIBAE COST ES0806
  EC; COST Office, Brussels, Belgium Asst. Prof. Sonja Lojen
  15. Conditioning of Drinking Water with Constructed Wetlands WETPUR
  EUREKA 3211-08-000211, S080067
  Limnos Company for Applied Ecollogy Ltd., Great Britain Prof. Janez Ščančar
- Francisco of Lung Cancer Caused by Radon Gas in Azerbaijan and Slovenia SCOPES

CCR-067, 127917

Dr. Claudio Valsangiacomo, Marcus Hoffmann, Swiss University of Applied Sciences of Southern Switzerland, Scuola Universitaria Professionale della Svizzera Italiana - SUPSI, Radon Competence Centre, Trevano, Canobbio, Switzerland; SNSF- Swiss National Science Foundation, Bern, Switzerland Dr. Chingiz Alyiev, Geology Institute of National Academy of Science, Baku, Azerbaijan

- Prof. Janja Vaupotič17. EMRP Emerging Requirements for Measuring Pollutants from Automotive Exhaust Emissions PartEmission
  - EMRP

ENV02

EURAMET e.V., Braunschweig, Germany; PTB - Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

- Prof. Milena Horvat Traceable Measurements for Monitoring Critical Pollutants under the European Water
- Framework Directive
- WFD-2000/60/EC
- EMRP

ENV08 EURAMET e.V., Braunschweig, Germany; Rosemarie Philipp, Bundesanstalt fuer

Materialforschung und-pruefung, Berlin, Germany

- Prof. Radmila Milačič
- Assessment of Human Milk Intake in Infants Living in Gold Mining Areas in South West Nigeria, Using Stable Isotope Techniques
  - 16475/R0, R1
  - IAEA, Vienna, Austria Dr. Darja Mazej
- 20. Use of Environmental Isotopes in Investigations of Influence of Snow Melt on Stream Runoff in the Area of Julian Alps, NW Slovenia
  - 16199/R0, R1
  - IAEA, Vienna, Austria
  - Dr. Polona Vreča
- 21. Stable Isotope Technique to Assess Human Milk Intake in Infants Living in Areas Contaminated with Mercury, Lead and Cadmium; Stable Isotope Technique to Assess Human Milk Intake in Infants Living in Contaminated Areas 15825/R0, R1, R2
  - IAEA, Vienna, Austria
  - Prof. Milena Horvat
- 22. IAEA Fellowship for Mr Fahti M. Zubeir
  - IAEA Fellow, LIB/10001, Pr. LIB/4/011
  - IAEA, Vienna, Austria
  - Dr. Radojko Jaćimović, Darko Kavšek, B. Sc.
- 23. Grant for "International Symposium on Isotopes in Hidrology, Marine Ecosystems and Climate Change Studies", Monaco, 27.3.-1.4.2011
  - IAEA, Vienna, Austria Saša Zavadlav, B. Sc.
- 24. Application of Advanced Methods in Determination of Geographic Origin of Wine: Comparison of Austrian and Slovenian Wine BI-AT/11-12-008
- Dr. Micha Horacek, Austrian Institute of Technology GmbH, AIT Business Unit Environmental Resources and Technologies, Seibersdorf, Austria Prof. Nives Ogrinc
- Batch Characterisation Measurements for ERM-CE278k Mussel Tissue IRMM.B058879
   European Commission, Joint Research Center JRC, Institute for Reference Materials and Magnetizements (JINM). Cool. Relation
- Measurements (IRMM), Geel, Belgium Dr. Radojko Jaćimović, Prof. Milena Horvat 26. Characterisation of Major and Trace Elements in Three Coal Materials by Activation
- Characterisation of Major and Trace Elements in Three Coal Materials by Activation and/or Destructive Methods IRMM.B058869

European Commission, Joint Research Center JRC, Institute for Reference Materials and

Measurements (IRMM), Geel, Belgium Prof. Milena Horvat, Dr. Radoiko Jaćimović

27. Determination of Total Content of Arsenic, Cadmium, Copper, Mercury, Lead, Selenium

and Zinc in ERM-DB001 (Human Hair)

IRMM.B058292 European Commission, Joint Research Center JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium

Dr. Radojko Jaćimović, Prof. Milena Horvat

28. Determination of Total Content of Arsenic, Cadmium, Copper, Mercury, Lead, Selenium and Zinc in ERM-CD200 (Fucus Vesiculosus) IRMM.B058275

European Commission, Joint Research Center JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium

- Dr. Radojko Jaćimović, Prof. Milena Horvat
- 29. Stability Monitoring of Al, Cd and Cu in BCR-060 Aquatic Plant IRMM.B058088

European Commission, Joint Research Center JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium

- Dr. Radojko Jaćimović, Prof. Radmila Milačič
- 30. ERM-CA713 Trace Elements in Wastewater (Characterisation Study) IRMM.B058239 European Commission, Joint Research Center JRC, Institute for Reference Materials and
  - Measurements (IRMM), Geel, Belgium Prof. Milena Horvat, Prof. Janez Ščančar
- 31. Stability Monitoring of BCR-463, ERM-CE464 and ERM-CC580 IRMM.B057275

European Commission, Joint Research Center JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium Prof. Milena Horvat

32. Homogeneity Study ERM-CC144. Total and Aqua Regia (according to ISO 11466) Extractable Content of As, Cd, Co, Cr, Cu, Fe, Hg, Mn, Ni, Pb and Zn in 14 Bottles of Sewage Sludge Candidate Reference Material ERM-CC144 IRMM.B056774 European Commission, Joint Research Center JRC, Institute for Reference Materials and

Measurements (IRMM), Geel, Belgium

Prof. Milena Horvat, Prof. Radmila Milačič 33. Stability Monitoring of ERM-CE477: 12 Measurements each of Monobutyltin (MBT), Dibutyltin (DBT) and Tributyltin (TBT) in the Reference Material ERM-CE477 IRMM.B057223 European Commission, Joint Research Center JRC, Institute for Reference Materials and

Measurements (IRMM), Geel, Belgium Prof. Janez Ščančar

34. Long-term Stability Study of ERM-CC141: Aqua Regia Content of Hg in Loam Soil; Aqua Regia Extraction, Determination of Hg by CV AAS according to the Guidelines on Longterm Stability Measurements of ERM-CC141 IRMM.B056527

European Commission, Joint Research Center JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium

- Prof. Milena Horvat
- 35. Training in Radiochemistry and Radioactivity Measurements for Practitioners from Countries Eligible under the JRC Enlargement & Integration Policy C59072

European Commission, Joint Research Center JRC, Institute for Reference Materials and Measurements (IRMM), Geel, Belgium

Asst. Prof. Ljudmila Benedik, Prof. Borut Smodiš

36. Applications of GIS Tools on Predermined Uranium Radioisotopes in Groundwater and Surface Water of Hadzici Region BI-BA/10-11-013

Alfred Vidic, B. Sc., Institute for Public Health of FB&H, Sarajevo, Bosnia and Herzegovina

- Asst. Prof. Ljudmila Benedik
- 37. Radilogical Investigation of Areas with Potentially Enhanced Levels of Natural Radionuclides BI-BA/10-11-019

Bojan Štrbac, M. Sc., Institut za zaštitu zdravlja Republike Srpske, Banja Luka, Bosnia and Herzegovina Prof. Borut Smodiš

38. Biogeochemistry of Mercury in Contaminated Coastal Environments; Coastal Lagoons in Rio Grande do Sul, Brazil and the Gulf of Trieste, Northern Adriatic BI-BR/10-12-001

Prof. Gilberto Fillmann, University of Rio Grande - FURG - Brazil, Rio Grande - RS -Brazil

Prof. Milena Horvat

39. Neutron Activation Analysis on the Assessment of Arsenic Resistant Plants from Santa Barbara Region, Iron Quadrangle, Brazil BI-BR/10-12-002

Dr. Maria Angela Menezes, Nuclear Tehnology Development Center / Brazillian Commission for Nuclear Energy, (CDTN/CNEN), Belo Horizonte, Minas Gerais, Brazil Dr. Radojko Jaćimović

Radiochemical Methods for Determination of Radionuclides in Water Samples 40.

BI-HR/10-11-007

- Dr. Martina Rožmarić Mačefat, Ruđer Bošković Institute, Zagreb, Croatia Asst. Prof. Ljudmila Benedik
- 41. Preparation of Environmental Samples for I-129 Determination with Accelerator Mass Spectrometry

BI-JP/10-12/A-004 Dr. Suzuki Takashi, Japan Atomic Energy Agency, Aomori, Japan

- Dr. Andrei Osterc 42. Where Radon (Gaseous Soil Component) is coming from?
- BI-JP/10-12-002 Asst. Prof. Ryoko Fujiyoshi, Hokkaido University, Graduate School of Engineering, Division of Quantum Science and Engineering, Sapporo, Japan Prof. Janja Vaupotič
- 43. Biomarkers of Exposure and Effects in Sensitive Population Groups Living in Contaminated Sites

BI-CN/09-11-007 Prof. Chunying Chen, Key Lab for Nuclear Analytical Techniques, Insitute of High Energy Physics (IHEP), Chinese Academy of Sciences (CAS), Beijing, China Prof. Milena Horvat

44. Environmental Impacts and Restoration after Closure of Wanshan Mercury Mine, Guizhou Province, China and the Comparison with Idrijca Mercury Mine, Slovenia BI-CN/09-11-025

Dr. Feng Xinbin, State Key Laboratory of Environmental Geochemisty, Institute of Geochemistry, Chinese Academy of Science, Guiyang, China Dr. Jože Kotnik

- 45. Effect of Short Lived Thoron Progeny on Effective Dose at Dwellings and Workplaces in Slovenia and Hungary
  - BI-HU/11-12-006 Prof. Tibor Kovács, University of Pannonia, Department of Information Systems, Veszprém, Hungary

Prof. Janja Vaupotič

46. Determination of Radilogical Situation at the Areas with Elevated Natural Radiation in Slovenia and in Poland BI-PL/10-11-006

Dr. Krzysztof Kozak, Institute of Nuclear Physics, Polish Academy of Science, Kraków, Poland

Prof. Janja Vaupotič

Development of Isotopic Tools for better Understanding of Impacts of Sava and Danube 47. Rivers on Groundwater Systems in Slovenia and Slovakia: Better Management of Groundwater Resources and their Protection Against Contamination Razvoj izotopových prostriedkov pre lepšie pochopenie dopadu riek Sava a Dunaj na Systémy podzemných vôd v Slovinsku a na Slovensku: Lepší manažment zdrojov podzemných vôd a ich ochrana proti kontaminácii BI-SK/11-12-005

Prof. Pavel Povinec, Faculty of Mathematics, Physics and Informatics of the Comenius University, Bratislava, Slovakia Prof. Nives Ogrinc

48. Hydrogeochemistry of Carbonate Weathering Fluxes at the Terrestrial/Marine Interface of the Adriatic Sea: A Collaborative Field Study BI-US/09-12-015

Prof. Walter Lynn M., University of Michigan, Geological Sciences, Ann Arbor, MI, USA Prof. Nives Ogrinc

# **R & D GRANTS AND CONTRACTS**

1. Chemical and biological cycling of endocrine disrupting compounds in wastewater treatment Prof. Janez Ščančar

Assessment of the risk from metal contaminated soils and aerosols to human health through advanced in vitro gastrointestinal and respiratory bioaccessibility tests Asst. Prof. Zdenka Šlejkovec

- Physicochemical Processes Involved in Formation of Radioactive Nanoaerosols 3. Prof. Jania Vaupotič
- Interaction of organic matter with metals in coastal waters of the Gulf of Trieste 4. Prof. Milena Horvat
- 5. The use of isotope dilution inductively coupled plasma mass spectrometry technique in environmental studies Prof. Radmila Milačič
- Synthesis, characterisation and use of novel ruthenium compounds in 6 electrochemotherapy of tumors (basic research project) Prof. Janez Ščančar
- Toxic metals and organometallic compounds in the terrestrial environment Prof. Radmila Milačič
- 8 Speciation and interactions of chemical contaminants at trace level in aqueous media to support the developement of cost-effective removal technologies Prof. Milena Horvat
- Influence of arsenic trioxide metabolites on treatment of various cancer types 9. Asst. Prof. Zdenka Šlejkovec



- 10. Afforestation of karstic grasslands and the changes of their carbon sink capacity Prof. Nives Ogrinc
- 11. The effect of selenium on the harvest and quality of crops Prof. Vekoslava Stibilj
- 12. Tartary buckwheat as a new source for functional foods Prof. Vekoslava Stibilj
- Sustainable land use in relation to soil and crop quality Prof. Nives Ogrinc
- 14. Metagenomics for bioexploration and biomining of bacterial laccases for a sustainable environment
- Prof. Ester Heath15. Archaeologies of hunter-gatherers, farmers and metallurgists: Cultures, populations, palaeoeconomies and climate
- Prof. Nives Ogrinc 16. Advanced water treatment with ultrasound and cavitation
- Prof. Ester Heath 17. An integrated methodology for the remediation of an area impacted by the past mining
- activity Prof. Milena Horvat
- Natural hydrochemical background and dynamics of groundwater in Slovenia Dr. Jasmina Kožar Logar
- 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 Milačič
- Modelling of hydrodynamics, sediment transport and sediment bound pollutants using the SPH method Prof. Milena Horvat
- 22. Optimisation of a polychlorinated biphenyls' (PCBs) contaminated material dump site remediation
- Dr. Andrej Stergaršek
- Petrology of brown (low-rank) coals as mined and/or used in Slovenia, natural gasses in them, and their gas-sorption properties Dr. Tiaša Kanduč
- 24. Climate change and impacts of anthropogenic disturbances on primary production in forest soil
- Prof. Nives Ogrinc 25. Carbon dynamics in forest soils and the rhizosphere
- Prof. Nives Ogrinc
- 26. The impact of climate change on the sustainability, stability and biodiversity of beech and black pine stands in the Balkans Prof. Nives Ogrinc
- Efficiency of SEA and Health Impact Assessment in Strategic Evaluation of Plans and Prof. Branko Kontić
- 28. The faith and speciation of pollutants in the transformation of contaminated biomass into synthetic fuel and pure hydrogen Dr. Andrej Stergaršek

- 29. Comparison of Two Production Forest Systems in the Light of Climate Change Prof. Nives Ogrinc
- 30. Farming Possibilities in Water Protection Areas Asst. Prof. Sonja Lojen
- The use of specific methods for determination and prevention of adulteration of milk and dairy products
- Prof. Nives Ogrinc
  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: competitive fisherm Prof. Vekoslava Stibilj
- 33. Sequestration of CO2 in geological media: criteria and approach for site selection in response to climate change Dr. Tjaša Kanduč
- Vulnerability assessment and identification of suitable remediation measures in degraded ecosystem – a case study of the Idrija mercury mine region Dr. David Kocman
- 35. Psychoactive pharmaceuticals and their transformation products in water treatment processes

Dr. Tina Kosjek

### 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

## NEW CONTRACTS

- Measurements of Hg in precipitation and elemental Hg in 2011 and 2012 Iskrba Ministry of the Environment and Spatial Planning Dr. Jože Kotnik
- Consultancy on environmental impact evaluations related to planned NPP2 Krško Gen d. o. o.
  - Prof. Branko Kontić
- Human biomonitoring of chemicals and their residues 2011-2012 Ministry of Health of the Republic of Slovenia Prof. Milena Horvat
- Co-financing of activities of holder of national standard in 2011 amount of substance / soil

Ministry of Higher Education, Science and Technology Dr. Polona Vreča

 Monitoring of the quality of the Slovenian surface and sea waters, sediments adn biota Ministry of the Environment and Spatial Planning Dr. Tea Zuliani

# MENTORING

### Ph. D. Theses

- 1. Tanja Ljubič Mlakar, Mercury in the process of cement clinker production and emission control (mentor Milena Horvat).
- 2. Larisa Pograjc, Impact of nutrition and physical stress on selenium status at soldiers (mentor Vekoslava Stibilj; co-mentor Ingrid Falnoga).
- 3. Marko Štrok, Migration of critical radionuclides in the area of former uranium mine Žirovski vrh (mentor Borut Smodiš).
- 4. Martina Šturm, Nitrate migration in plant-soil-groundwater sistem (mentor Sonja Lojen).
- Mitja Vahčič, Development of analytical methods for speciation of organotin compounds in environmental samples using gas chromatography and mass spectrometry (mentor Janez Ščančar).
- Urška Zapušek Novak, Preparation of artificial soil mixtures with sewage sludges (mentor Domen Leštan; co-mentor Radmila Milačič).

### M. Sc. Thesis

 Cândida Radicchi de Oliveira Alméri, Environmental impacts of aluminium and chromium in bauxide ore and red mud (mentor Janez Ščančar; co-mentor Radmila Milačič).

### VISITORS FROM ABROAD

- 1. dr. Martina Rožmarić Mačefat, Rudjer Bošković Institute, Zagreb, Croatia, 24-27 January 2011
- 2. prof. Gaetane Lespes, dr. Maité Bueno, University of Pau, Pau, France, 17-21 January 2011
- dr. Claudio Valsangiacomo, dr. Marcus Hoffmann, Radon Competence Centre, University of Applied Science of Southern Switzerland (SUSPI), Trevano, Switzerland, 20-22 January 2011
- 4. dr. Robbert van Sluijs, k0-ware, Heerlen, Heerlen, Netherlands, 14-15 February 2011
- 5. dr. Yan Haiyu, Liu Bian, Institute of Geochemistry, Guiyang, China, 7-12 May 2011
- 6. dr. Marijana Zanoški, University of Zagreb, Zagreb, Croatia, 1 February to 30 April 2011
- dr. Zora Žunić, prof. dr. Ivan Aničin, prof. dr. Jovan Puzović and dr. Vladimir Udovičić, Vinča Institute of Nuclear Sciences, Faculty of Physics, University of Belgrade, Belgrade, Serbia, 6-10 March 2011
- Michal Emilian Miotk, Institute of Oceanology PAS, Sopot, Poland, 28 February to 11 March 2011
- 9. dr. Sergio Ribeiro Guevaro, Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Bariloche, Argentina, 14 March to 1 April 2011
- dr. Eliana Knupp, dr. Maria Eleonora Carneiro, dr. Lucia Maria Auler and dr. Maria Angela Menezes, CDTN/CNEN, Belo Horizonte, Brazil, 25 March to 2 April 2011
- dr. Tibor Kovács, Borbála Máté, Maria Horváth and dr. Richárd Kardos, Institute of Radiochemistry and Radioecology, Pannonian University, Veszprem, Hungary, dr. Yosuke Kobayashi, National Institute of Radiological Sciences (NIRS), Inage, Chiba, Japan 30-31 March 2011
- dr. Micha Horacek, Stefan Wyhlidal, Andrea Watzinger, AIT Austrian Institute of Technology GmbH, Seibersdorf, Austria, 31 March to 1 April 2011
- 13. dr. Martina Rožmarić Mačefat, Rudjer Bošković Institute, Zagreb, Croatia, 25-28 April 2011

- 14. dr. Richárd Kardos, Institute of Radiochemistry and Radioecology, Pannonian University, Veszprem, Hungary, 13 April to 5 May 2011 15. dr. Claudio Valsangiacomo, dr. Marcus Hoffmann, dr. Luca Pampuri, Radon
- Competence Centre, University of Applied Science of Southern Switzerland (SUSPI), Delémont, Switzerland, 4-7 May 2011
- 16. dr. Yan Haiyu, Liu Bian, Institute of Geochemistry, Guiyang, China, 7-12 May 2011
- 17. dr. Kathrin Szramek, Drake University, Des Moines, Iowa, USA, 18 May to 8 June 2011
- 18. dr. Jadwige Mazur, dr. Krzysztofa Kozaka and mag. Dominika Grządziela, Laboratory of Radiometric Expertise, Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland, 30 May to 9 June 2011
- 19. dr. Martina Rožmarić Mačefat, Matea Rogić, Rudjer Bošković Institute, Zagreb, Croatia, 17-19 July 2011
- 20. dr. Pavel Povinec, Comenius University of Bratislava, Bratislava, Slovakia, 28 August to 3 September 2011
- 21. prof. dr. Vitaliy Rusov, prof. dr. Tetiana Zelentsova, Volodymyr Smoliar, Odessa National Polytechnic University, 2-30 September 2011
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- 25. dr. Alexey Ekaykin, Arctic and Antarctic Research Institute, St. Petersburg, Russian Federation, 10-20 October 2011

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- 28. prof. dr. Ryoko Fujiyoshi, Y. Sakuta, T. Okabayashi, Hokkido University, Sapporo, Japan, -17 September 2011
- 29. dr. Weng Weiguo, Zhejiang University LCEU, Hangzhou, China; Mr. Chen, Jian, Zhejiang Xizi United Engineering Co., Ltd ; Mr. Jiang, Shanxing, Hangzhou Beigaofeng Power Engineering Design Co., Ltd; Mr. Zhang, Yongxin, Process Engineer, Zhejiang University; Mr.Wu, Weihong, Process Engineer, LAN-TIAN Environmental Engineering Co., Ltd; Ms. Xu, Dian, Process Engineer, Zhejiang University; Dr. Gao, Xiang, Department of Energy Engineering, Zhejiang University, China, 9-11 November 2011
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- 32. dr. Claudia Valsangiacoma, Radon Competence Centre, University of Applied Science of Southern Switzerland (SUPSI), Canobbio, Switzerland, 11 November 2011
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- 34. Cristian Nicolae Dulama, Institute for Nuclear Research, Pitesti, Romania; Elena Simion, National Environmental Radioactivity Laboratory, Bucharest, Romania; Ruxandra Toma, Logofat Stanciu Mihoveanu, Mioveni, Romania; Gergana Rumenova Ivanova, Jivko Gospodinov Tenev, National Center of Radiobiology and Radiation Protection, Sofia, Bulgaria, 21 November to 2 December 2011

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### **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

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- 2. Thomas Breznik, Marko Gerbec, Borut Smodiš, "Task analysis and risk assessment of the transport of the radioactive material by road in the Republic Slovenia", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 8 pp., 2011.
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- 4. Asta Gregorič, Janja Vaupotič, "Diurnal variation of radon concentration in the Postojna cave", In: *Zbornik radova VIII. simpozija Hrvatskog društva za zaščitu od zračenja: HDZZ - CRPA: Zagreb 2011*, Ines Krajcar Bronić, ed., Zagreb, Hrvatsko društvo za zaščitu od zračenja, 2011, pp. 238-242.
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- 18. Tina Oblak, Radmila Milačič, Janez Ščančar, "Razvoj analiznega postopka za določanje kroma v morski vodi z ICP-MS", In: *Slovenski kemijski dnevi 2011, Portorož, 14-16 september 2011*, Zdravko Kravanja, ed., Darinka Brodnjak-Vončina, ed., Miloš Bogataj, ed., Maribor, FKKT, 2011, 8 pp.
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- Sonja Lojen, Nives Ogrinc, The use of tracers in the environment: "Ecotechnoloy" programme, fall semester 2010/11, (Postgraduate courses in ecotechnology), Ljubljana, Jožef Stefan International Postgraduate School, 2011.
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- 12. Borut Smodiš, Radioaktivnost, radionuklidi, detekcija in meritve, radiokemija, tritij: Storitve kemičnega in biološkega laboratorija, Ministrstvo za obrambo RS, 2011, Ljubljana, 2011.
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- 15. Janez Ščančar, Radmila Milačič, *Elements in the environment: fall semester 2011/2012*, (Postgraduate courses in ecotechnology), Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011.
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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 is optimising the "behaviour of man and machine", accounting for the interaction with the environment. By combining engineering sciences and life sciences, we have been able to make significant contributions to the development of: 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 the field of production technologies. The Programme Group has three major overlapping research Head:

foci: automation and intelligent control, humanoid and cognitive robotics, and biocybernetics. Asst. Prof. Leon Žlajpah By maintaining a critical mass of researchers in all three areas within one Programme Group, we have managed to foster exciting multidisciplinary projects.

During the past year, the main research topics in the department included humanoid robotics, control of robot systems and learning strategies, studies of human physiology in extreme environments, evaluation of protective equipment, 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 automation of industrial processes.

Historical note: Since its inception the department has maintained an inter- and multidisciplinary research focus. The scientific inheritance of its founders includes pioneering research culminating in the first demonstration of how functional electrical stimulation can assist paraplegics to walk, and the development of the first industrial robots in our region. In addition to kinematics, the common denominator in the biomedical and robotic research is improving the quality of life.

### Advanced robot control

Our research into the methods for controlling rhythmic robotic tasks led us to new methods of extracting frequencies of the movement for the tasks that require synchronization. We proposed an improvement of the method

based on nonlinear oscillators. The method allows straightforward synchronization with the controlled object and intuitive supervised robot learning for performing rhythmic tasks. We published the results in the prestigious scientific journal The International Journal of Robotics Research, which is the top-ranking journal in the field of robotics. We applied the method to different tasks, such as controlling the yo-yo, cooperative human-robot rope turning, synchronization with human movement using EMG and human synchronization using electrical stimulation. The applications demonstrate the robustness and usefulness of the proposed method.

In the field of kinematically redundant robots we developed methods, which allow prioritized control of robots with the possibility of continuous and reversible transition between tasks. The method works in a reflexive manner - only when necessary. The developed method can be applied to different tasks, such as reflexive maintenance of stability, and also for obstacle avoidance. We applied the method to different mechanisms. On the mechanism of the humanoid robotic leg we demonstrated how it can be Figure 1: Dr. Ude announcing one of the Humanoids 2011 plenary applied for reflexive stability. We applied the same method to a skiing robot. speakers, prof. Mitsuo Kawato



A new method of extracting frequencies of movement for the tasks that require synchronization has been published in the prestigious scientific journal The International Journal of Robotics Research. The method allows the maintenance of a desired skiing trajectory while the robot is stable, but when the maintenance of the desired trajectory would tip the robot over, the method ensures stability, sacrificing the direction of skiing. These different tasks are all incorporated in a single system of kinematic equations.

We also developed a new dynamic model of the skiing robot. The model allows a simulation with hardware-in-the-loop. The previously mentioned

reflexive stability algorithm was tested with the parallel Stewart platform. We also improved the detection of gates by the skiing robot by incorporating simultaneous localization and mapping (SLAM) algorithms.

### Robot motion synthesis through human sensorimotor learning

In the context of robot motion synthesis that exploits human capability of sensorimotor learning, we investigated the role of proprioceptive-vestibular and visual feedback during human motion. We performed a series of



Figure 2: Part of our research in PACO+ and Xperience is conducted in collaboration with ATR Computational Neuroscience Laboratories, Kyoto, Japan. The picture shows our joint experiments on object learning by manipulation.

experiments, whereby human subjects controlled, in real-time, a humanoid robot with the motion of their own body. We focused on the feedback connection between the robot and the human that is necessary for keeping the humanoid robot balanced. We discovered that the capability of the control is significantly higher when human subjects receive the feedback information regarding the robot's postural balance with the proprioceptive-vestibular senses, than with the visual feedback connection. In addition, we developed an adaptable machine learning algorithm, which maintains the balance of a humanoid robot based on the feedback flow of information from the robot to the human. By doing this, we would like to transfer the computational processes in the human central and peripheral nervous system that are responsible for keeping the postural balance of the robot from the human side to the robot side.

### Full-body optimum human motor control

Within the framework of our research of motor-control principles used by the human brain for the control of full-body motion, we continued with an extensive study of human motion. We used a novel experimental approach, where we induced external postural perturbations to the subjects during their execution of a prescribed motion. During the repetitions of the prescribed motions, the subjects used their learning ability to compensate for the postural perturbations. We recorded the motion of the subjects during this adaptation and analysed the obtained trajectories. Using this approach, we achieved an adaptation of the central and peripheral nervous systems

to a novel and precisely determined environment which gave us a systematic insight into the neural mechanisms responsible for learning the body motions. A comparison of our results with those previously reported on for the motor control principles and the learning of arm movements, revealed that humans do not use the same strategy for moving the arms and for moving the body.

In October 2011 we organized, what is considered to be the most prestigious scientific conference in the field of humanoid robotics, and the first such conference ever organized in Slovenia: 2011 11th IEEE-RAS International Conference on Humanoid Robots (Humanoids 2011).

### Confidence

Within the European Framework Programme 7 project "Ubiquitous Care System to Support Independent Living" (CONFIDENCE) we completed a project on the detection and recognition of abnormal events (such as falls) or unexpected behaviours that might be related to a health problem in the elderly. We measured the motions of individuals during different daily activities and during abnormal behaviour, such as characteristic falls or motion influenced by typical pathologies associated with the elderly. This information was then used in a system with an advanced functionality for the supervision of the elderly.

### Automation, robotics and factory information systems for manufacturing

In 2011, we continued our cooperation with the company Steklarna Hrastnik that manufactures a large range of glass products. Last year we studied, designed and developed various dedicated automation components, about which we learned that they can be used not only for our current automation task, but also for our future automa-

tion R&D work in the target glass production environment. In order to achieve this, these components were adequately conceived, designed and developed in a distinctly modular and reusable form. These components mainly include program modules and also hardware subsystems. These were used for various prototype systems we developed, for example, in a system for automated execution of a glass forming operation, and in a number of measurements and analysis subsystems, designed to support the formalization and quantification of the current manual operations. All these activities are important steps in the applied research, experimental and development work, targeted to the automation of glass forming operations.

### Humanoid and Cognitive Robotics



The aim of the research within this group 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 them than with other types of robots. We therefore believe that a cognitive humanoid robot is 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.

Our research has been an integral part of international research activities in this area for many years. In 2011 our group was therefore entrusted to host the largest and most important event in humanoid robotics worldwide: 11th IEEE-RAS International Conference on Humanoid Robots (Humanoids 2011). Previous conferences were organized by leading world centres for humanoid robotics (MIT, CMU, Karlsruhe Institute of Technology, Waseda, etc.). The conference was attended by over 250 researchers from all over the world, among them many of the most distinguished scientists in the field. The papers and posters were thoroughly peer-reviewed to ensure the highest quality of the presented papers. Members of our group were the

key organizers, among them dr. Aleš Ude as the conference general chair, dr. Bojan Nemec as the financial chair, and dr. Andrej Gams as the publication chair. The conference was sponsored by public and private entities includ-

ing euCognition project, Slovenian Research Agency, Aldebaran Robotics, Robotnik, Barret Technology, and PAL Robotics. More details can be found at http://www.humanoids2011.org/.

The humanoid and cognitive robotics group is involved in a number of EU projects within the programme "Cognitive Systems and Robotics". In 2011 we successfully completed a large-scale integrated project "Perception, action, and cognition through the learning of object-action complexes" (PACO+, IST-FP6-IP-027657), which included 10 collaborating partners. PACO+ was immediately followed by a launch of two new FP7 projects funded by the same programme:

- 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.

### PACO+ (http://www.paco-plus.org/)

The main result of PACO+ is the formalization of object-action complexes (OACs) as the basis for symbolic representations of sensorimotor experience and behaviour. OACs are designed to capture the interaction between objects and associated actions in artificial cognitive systems. The OAC concept can be used to bridge the gap between low-level sensorimotor representations, required for robot perception and control, and high-level representations supporting abstract reasoning and planning. As such it provides a grounded formalism that is of great importance for the development of embodied cognitive systems. We demonstrated within the project how OACs operate and interact with other OACs, and also how OACs can be learnt by robotic systems.

Figure 3: Application of obstacle-avoidance algorithm as a primary task on a two-arm robot, following the motion of a human demonstrator. The algorithm assures that during the tracking of the demonstrator's motion no collision between the arms occurs.

Two new FP7 projects were initiated within the EU Framework Programme 7 "Cognitive Systems and Robotics": a large-scale integrated project "Robots bootstrapped through learning from experience" and the specific targeted research project "Intelligent observation and execution of actions and manipulations".



Figure 4: Experimental setup for studying the role of proprioceptivevestibular and visual feedback connections during the control of the postural balance of the humanoid robot

### *Xperience* (http://www.xperience.org/)

Current artificial cognitive systems are limited with respect to the generative mechanisms that rely on prior knowledge. They are employed to predict the immediate future and are of key importance in 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



Figure 5: Assessment of blood flow (with Doppler ultrasound) in the mesenteric artery following a standard meal, during exposure to a simulated altitude of 3400 meters.

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 introspective, predictive, and interactive understanding of actions and dynamic situations. In the first year of the project we developed new methodologies for long-term robot sensorimotor learning. The developed behaviours can provide grounded experiences needed to generate new knowledge via structural bootstrapping.

### *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 movements of the human but by transferring the human action to the semantic level. IntellAct will demonstrate the ability 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. In the first year of the project we developed

new technologies for action observation and segmentation and a new paradigm for robot learning that integrates imitation learning and reinforcement learning.

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. All these projects focus on 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 this group focused primarily on the projects concerning the influence of extreme environments on humans, and evaluation of technology and strategies to maintain 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. This required the establishment of a Planetary Habitat Simulation Facility, initiating research investigating the effect of such environments on homoestatic mechanisms in humans. The partial pressure of oxygen of the ambient air in future planetary habitats will be lower than in the atmospheric air. Prolonged exposure to low gravity will result in 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. The new knowledge also has implications for the society in general, since chronic hypoxia and bedrest constitute a model of the basic conditions experienced by patients suffering from respiratory insufficiency restricting them to a physically inactive life style. The challenge of the project lies in the complexity of the experimental interventions, where healthy humans are confined to a hypoxic environment during a prolonged bedrest. A series of studies funded by the European Space Agency Programme for European Participating Countries have been completed at the Planica hypoxia facility. The subjects 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.

### Hypoxia and weight loss

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 our knowledge, no systematic studies have been carried out to date regarding the treatment of obesity under hypoxic conditions. The mechanism of weight loss is not entirely due to an imbalance between energy intake and expenditure. During longer exposures to higher altitudes, factors which may contribute to weight loss, include: primary anorexia, lack of comfort and palatable food, detraining, and possibly direct effects of hypoxia on metabolism. We have completed a series of studies investigating the effect of 10-d sojourns in hypoxia, equivalent to a simulated altitude of 3,200 m, on 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.

### Mathematical model of human temperature regulation

In collaboration with Professor Eugene Wissler and industrial partner Biomed d.o.o., we modified the Wissler Mathematical Model of Human Temperature Regulation to account for the characteristics of the clothing layer. This modification allowed the simulation of scenarios such as maritime accidents. Specifically, the model was used to predict the survival time during an immersion of unconscious victims in cold water. The simulations were validated with human experiments conducted by the Royal Institute of Technology (Stockholm, Sweden).

### Planica protocol for the treatment of freezing cold injury

Frostbite is a local cold injury that may lead to loss of tissue and result in disability. It is normally a consequence of a prolonged exposure of unprotected regions to subzero ambient temperatures, which causes impairment of the microcirculation. In Slovenia, the main risk group for frostbite injury are mountain climbers. Frostbite is classified as either a superficial-reversible injury, or a deep irreversible tissue injury. Superficial frostbite is managed in out-patients clinics, whereas hospital treatment is required for deep frostbite. The success of frostbite management depends a great deal on the field first



Figure 6: Using infrared thermography to monitor the hand and foot digits following an immersion in cold water, we have been able to classify individuals into high- and low-risk groups for cold injury.

aid and emergency medical treatment, as well as the subsequent hospital treatment. Together with researchers from the University Clinical Centre Ljubljana we have developed a protocol (Planica Protocol) for hospital treatment of frostbite, comprising the early diagnosis with three-phase bone scintigraphy (TS), administration of appropriate medications, particularly iloprost, and initiation of hyperbaric oxygen treatment (HBOT).

### Development of 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 the researchers from the Royal Institute of Technology (Stockholm, Sweden), we have initiated a research programme, which has two specific aims: i) develop a diagnostic method to determine the susceptibility of individuals to cold injury; ii) develop a training programme to improve individual's vascular response to a cold stimulus.

### **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. Our research programme initially focussed on the physiological responses of soldiers carrying loads in such environments. We have continued our work in this area, by evaluating the efficacy of different technologies and/or strategies in minimising heat strain and improving performance in such environments. As a member of the NATO Human Factors in Medicine Panel 187 "Thermal Strain Management for Health and Performance Sustainment", Prof. Mekjavic regularly conveys the results of this research to the established NATO task force.

### Some outstanding publications in the past three years

- 1. Tadej Petrič, Andrej Gams, Auke Jan Ijspeert, Leon Žlajpah. On-line frequency adaptation and movement imitation for rhythmic robotic tasks. Int. j. rob. res., Vol. 30, No. 14, p. 1775-1788, 2011.
- 2. Aleš Ude, Andrej Gams, Tamim Asfour, Jun Morimoto. Task-specific generalization of discrete and periodic dynamic movement primitives. IEEE trans. Robot.. [Print ed.], Vol. 26, No. 5, p. 800-815, 2010.
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- 4. Jan Babič, Joshua G. Hale, Erhan Oztop. Human sensorimotor learning for humanoid robot skill synthesis. Adapt. behav., Vol. 19, No. 4, p. 250-263, 2011.
- 5. Arne Tribukait, Gerard Nobel, Igor B. Mekjavic, Ola Eiken. Effects of anti-histaminic and anti-cholinergic substances on human thermoregulation during cold provocation. Brain res. bull. 81 (1): 100-106, 2010
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- Tadej Debevec, Michail E. Keramidas, Barbara Norman, Thomas Gustafsson, Ola Eiken, Igor B. Mekjavic. Acute short-term hyperoxia followed by mild hypoxia does not increase EPO production: resolving the "normobaric oxygen paradox". European Journal of Applied Physiology (in press) 2011.

### Organization of conferences, congress and meetings

8

- 1. Human factors & medicine (HFM) panel, Group meeting HFM-187: »Thermal strain management for health & performance sustainment, Planica, Slovenia, 5–7 March 2011 (team leader Igor B. Mekjavić)
- IEEE-RAS International Conference on Humanoid Robots HUMANOIDS 2011, Bled, Slovenia, 26–28 October 2011 (president Aleš Ude)

# INTERNATIONAL PROJECTS

- 1. Inteligent Observation and Execution of Actions and Manipulation
  - IntellÄct
  - 7. FP, 269959
  - EC; Syddansk Universitet, Odense, Denmark
- Asst. Prof. Aleš Ude
- 2. Robots Bootstrapped through Learning from Experience Xperience
  - 7. FP, 270273

EC; Karlsruhe Institute of Technology, Karlsruhe, Germany Asst. Prof. Aleš Ude, Prof. Matjaž Gams

- International Cooperation for the Advancement of Researcher on the Undrelaying System of Human Thermoregulation
  - ICARUS
  - 7. FP, 247631 EC
- Prof. Igor Mekjavić
- Ubiquitous Care System to Support Independent Living CONFIDENCE
- 7. FP, 214986
- EC; Centro de Estudios e Investigaciones Tecnicas de Guipuzcoa, San Sebastian, Spain Asst. Prof. Leon Žlajpah, Prof. Matjaž Gams
- 5. Planetary (Lunar & Mars) Habitat Simulations
  - PLANICA ESA PECS, 4000104372/11/NL/KML
  - Bernard Zufferey, ESA The European Space Agency, Paris, France; European Space Research and Technology Centre, Noordwijk, The Netherlands Prof. Igor Mekiavić
- IEEE-RAS International Conference on Humanoid Robots Humanoids 2011, Bled, Slovenia, 26-28.10.2011
   EUCogII Coordination Office, c//o Theodoros Gantinas, Anatolia College/ACT, Pylaia,
- Greece Asst. Prof. Aleš Ude
- Development of an Artificial Skin as Element of Sweating Thermal Manikin PROTEUS BI-FR/11-12-PROTEUS-004

Dr. Andre Dufour, LINC (Laboratory of Imagery and Cognitive Neuroscience), CNRS (National Centre for Scientific Research) & UdS (University of Strasbourg), Strasbourg, France

- Prof. Igor Mekjavić Development of Protective Clothing Systems - Numerical Modelling of Textile
- BI-HR/10-11-013 Dr. Anica Hursa, Tekstilno-tehnološki fakultet Sveučilišta u Zagrebu, Zagreb, Croatia Prof. Igor Mekjavić
- Source Code for Vision-based Control of the Humanoid Robot CB-i 0114-110214-003
   Dr. Mituue Kawato, Advanced Telecommunications Research Institut

Dr. Mitsuo Kawato, Advanced Telecommunications Research Institute International (ATR), Computational Neuroscience Laboratories, Kyoto, Japan Asst. Prof. Ude Aleš

- Co-financing of the Hypoxic and Hyperoxic Exercise Contract dtd. 16.4.2009
   Edwin Willemsen, b-Cat BV, Tiel, The Netherlands Prof. Igor Mekjavić
- Co-financing the Implementation of the Project entitled Zero and Reduced Gravitiy Simulation: The Effect on the Cardiovascular and Muskuloskeletal Systems Contract dtd. 30.6.2010

Royal Institute of Technology - KTH, School of Technology and Health - STH, Department of Environmental Physiology, Solna, Sweden Prof. Igor Mekiavić

# R & D GRANTS AND CONTRACTS

- 1. Dual nature of stem cells in cancer and their application in therapy Prof. Igor Mekjavić
- 2. Robot motion synthesis through human visuo-motor learning Dr. Jan Babič
- Goal directed action synthesis using a library of example movements Asst. Prof. Aleš Ude
- 4. Learning, analysis, and detection of motion in the framework of a hierarchical

compositional visual architecture Prof Roman Trobec

- The role of small GTPases in the regulation of endosomal/lysosomal transport in 5 astrocytes
  - Prof. Igor Mekjavić
- 6. The detection of irregularities and fraud in the financing of the public health services Asst. Prof. Rok Okorn
- 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
- Zero and reduced gravity simulation: the effect on the cardiovascular and 8. musculoskeletal systems Prof. Igor Mekjavić
- MENTORING

### Ph. D. Theses

- 1. Tadej Debevec, The use of normobaric hypoxia and hyperoxia for the enhancement of sea level and/or altitude exercise performance (mentor Igor B. Mekjavić; co-mentors Blaž Jereb, Stylianos N. Kounalakis).
- Michail Keramidas, Normobaric Hyperoxia: Haemodynamic responses to acute and long-term exposure (mentor Igor B. Mekjavić; co-mentors Ola Eiken, Nickos D. Geladas).

### Bologna M. Sc. Thesis

Jurij Gorjanc, The effectivity of cold induced vasodilatation as predicting factor for 1. freezing cold injury (mentor Metka Milčinski; co-mentor Igor B. Mekjavić).

### VISITORS FROM ABROAD

1. Prof. Marcia Riley, Technische Universität München, Germany, 27 February to 2 March 2011 Prof. Takaaki Kurate, Technische Universität München, Germany, 27 February to 2 2. March 2011

### STAFF

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- 1. Dr. Jan Babič
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- Dr. Ladislav Lenart 4.
- Prof. Igor Mekjavić 6.
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### 9. Asst. Prof. Leon Žlajpah, Head

### Postdoctorial associates

- 10. Dr. Mitja Babič
- 11. Dr. Gregor Cigler\*
- 12. Dr. Tadej Debevec
- 13. Dr. Andrei Gams
- 14. Dr. Michail Keramidas
- 15. Asst. Prof. Marjeta Kramar Fijavž\* 16. Dr. Shawnda Morrison
- 17. Dr. Martin Tomšič, left 01.05.11

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- 18. Mojca Amon\*, M. Sc.
- 19. Denis Forte, B. Sc.

- Hypoxic inactivity: Implications for heart failure, respiratory insufficiency and obesitas 9. Prof. Igor Mekiavić
- Influence of ski width on alpine skiing safety 10 Asst. Prof. Bojan Nemec
- 11. Hypoxic and hyperoxic exercise Prof. Igor Mekjavić
- 12. Biologically inspired synthesis of periodic movement for a robotic humanoid leg Dr. Andrei Gams

### RESEARCH PROGRAM

- 1. Avtomation, biocybernetics and robotics Prof. Jadran Lenarčič
- 3. Prof. dr. Ola Eiken, Department of Environmental Physiology, School of Technology and Health, Stockholm, Sweden, 21 March to 15 April 2011
- Dr. Kai Salminen, Tampere University of Technology, Finland, 19-22 April 2011 Prof. Ola Eiken, Department of Environmental Physiology, School of Technology and 5.
- Health, Stockholm, Sweden, 3- 26 May 2011
- 6. Prof. Minija Tamašiunaite, Vytautas Magnus University, Kaunas, Lithuania, 31 May to 2 June 2011
- 7. Prof. Ola Eiken, Department of Environmental Physiology, School of Technology and Health, Stockholm, Sweden, 10 June to 3 July 2011
- Prof. Ivan Godler, University in Kitakyushu, Japan, 8– 9 July 2011 Dr. Takashi Sonoda, IST Fukuoka, Japan, 8– 9 July 2011 8
- 9
- Dr. Michael Gronkvist, Department of Environmental Physiology, School of Technology 10. and Health, Royal Institute of Technology, Stockholm, Sweden, 21-28 September 2011 11 Prof. Nikos Geladas, Faculty of Physical Education and Sport Sciences, National and
- Kapodistrina University of Athens, Greece, 21-28 September 2011 12. Dr. Mikael Gronkvist, Department of Environmental Physiology, School of Technology
- and Health, Royal Institute of Technology, Stockholm, Sweden, 11 October to 30 November 2011
- Prof. Pietro di Prampero, Dipartimento di Scienza e Technologie Biomedicine 13. Universita di Udine, Italy, 23 September 2011
- 20. Nejc Likar, B. Sc.
- 21. Adam Mc Donnell, B. Sc.
- 22. Rok Okorn\*, B. Sc.
- 23. Luka Peternel, B. Sc.
- 24. Tadej Petrič, B. Sc.
- 25. Goran Škorja, B. Sc., left 01.10.11
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- 28. Miha Deniša, B. Sc.
- 29. Borut Lenart, B. Sc. 30. Juan Saez Pons, B. Sc., left 12.09.11
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- 36. Janez Zalar

Note: \* part-time JSI member

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- 3. Andrej Gams, Tadej Petrič, Leon Žlajpah, Aleš Ude, "Optimizing parameters of trajectory representation for movement generalization: robotic throwing", *Int. j. mech. control*, vol. 12, no. 1, pp. 19-25, 2011.
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1. Daniela Zavec Pavlinič, Jože Balič, Igor B. Mekjavić, "Determination of the thermoregulatory specifications for thermal manikins", In: *DAAAM International scientific book 2011*, (DAAAM International scientific book), Branko Katalinić, ed., Vienna, DAAAM International Publishing, 2011, pp. 31-44.

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- 1. Jan Babič, "Utilization of human sensorimotor learning capacity for obtaining novel robot behaviours: 2-DOF ball balancing on a parallel platform", In: *IEEE-ROBIO 2011*, [Piscataway], IEEE, cop. 2011, pp. 1778-1782.
- 2. Mitja Babič, Jadran Lenarčič, "Improvements of the electronic driver design for dielectric elastomer actuators", In: *Zbornik 14. mednarodne multikonference Informacijska družba - IS 2011, 10.-14. oktober 2011: zvezek A: volume A*, (Informacijska družba), Marko Bohanec, ed., Matjaž Gams, ed., Dunja Mladenić, ed., Marko Grobelnik, ed., Marjan Heričko, ed., Urban Kordeš, ed., Olga Markič, ed., Jadran Lenarčič, ed., Leon Žlajpah, ed., Andrej Gams, ed., Vladimir Fomichov, ed., Olga S. Fomichova, ed., Andrej Brodnik, ed., Rok Sosič, ed., Vladislav Rajkovič, ed., Tanja Urbančič, ed., Mojca Bernik, ed., Ljubljana, Institut Jožef Stefan, 2011, pp. 343-346.
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- 4. Tadej Debevec, Igor B. Mekjavić, "Oxygen breathing manipulations for enhancing erythropoietin producting", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 10-15.
- 5. Miha Deniša, Bojan Nemec, Aleš Ude, "Generation, generalization and adaptation of motion primitives", In: *RAAD 2011*, 20th International

Workshop on Robotics in Alpe-Adria-Danube Region, October 5-7, 2011, Brno, Czech Republic, [S. l., s. n.], cop. 2011, pp. 102-107.

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### TEXTBOOKS AND LECTURE NOTES

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### THESES

#### Ph. D. Theses

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#### B. Sc. Theses

- 1. Luka Peternel, *Navigation learning for skier robot:* undergraduate thesis, Ljubljana, [L. Peternel], 2011.
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# 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**

Basic and applied research in 2011 was devoted to three sub-areas: the methodologies for analysis and controlsystems design; the tools and building blocks for implementation; and the applied research in the priority problem domains.

as: the methodologies for analysis and controlnd the applied research in the priority problem **ms design** included three topics. The first topic **plex dynamical systems**. The research in the ted towards the incorporation of various prior

The sub-area **the methodologies for analysis and control systems design** included three topics. The first topic addressed the **modeling and identification of nonlinear and complex dynamical systems**. The research in the dynamic-systems modeling of the Gaussian-process models was directed towards the incorporation of various prior knowledge and model-optimization methods for dynamic-systems identification and the application of modeling with the Gaussian process models of traffic, process engineering and environmental systems. Performance analyses

of several algorithms for the joint state and the parameter estimation of the nonlinear dynamic systems have been accomplished. It turned out that the standard identification algorithms can fail in the case of low-dimensional systems. It seems that for higher-dimensional systems the estimation of the covariance parameters is the main cause for divergence problems.

The second topic was the (advanced) control. Within the research and development of explicit predictive controllers we have developed an efficient method of complexity reduction of the polyhedral controller partition using a dual sampling rate, and formed a systematic approach to reliable computation of the partition using the parametric linear complementarity algorithm for the numerically challenging problems and degeneracies (Figure 1). Research in the field of the PID control algorithms has been expanded to oscillatory systems, where a combination of the Magnitude Optimum Multiple Integration and the Posicast method has been proposed in order to decrease oscillations in the closed-loop system.

The third topic of interest was the condition monitoring and fault diagnosis. Research has been focused on the diagnostics and prognostics of mechanical drives under the non-stationary operating conditions. A novel

robust method for the detection of bearing faults based on the statistical-point processes has been proposed. The idea behind it is that the statistical pattern of the inter-event times between repetitive impacts depends, in major part, on faults and less on operating conditions. A new approach to an estimation of the remaining useful life (RUL) of the mechanical drives operating under non-stationary conditions was derived. It relies on an assumption that a fault can be treated as a hidden state of a dynamic process, while the transmitted power and the temperature are thought to be process inputs. The process is described by a linear model, whose parameters and states are estimated on-line in order to calculate the RUL horizon. We also developed the first prototype of a smart node for a wireless sensor network used for the on-line diagnostics and prognostics of industrial drives. The node performs data acquisition from the (micro)sensors installed on a drive and local signal processing, which results in the features being communicated to and stored on the server. The final diagnosis and prognosis are carried out on the server. One of the key ideas of the approach concerns the environment for the design of the application software in Matlab/Simulink and then an easy automatic conversion into the run-time code on the target smart node. The highly innovative approach is expected to significantly extend the applicability of the automated condition monitoring to a more efficient asset maintenance due to a powerful functionality that is less costly than the one currently used.

An important feature of the modern prognostics and health-management tools are their abilities to adapt to the changes in the operating conditions of the machine and an automatic update of the estimate and the prediction.



Figure 1: State-space partition of a parametric predictive controller

To this end, we have developed novel algorithms for an automatic on-line model learning that protect the robust systems from the changes in the operating conditions.

A part of the work, which is also related to the condition monitoring, dealt with the problem of monitoring



Figure 2: Nyquist plot of the impedance characteristics of the fuel-cells system under different operating conditions

Andrej Debenjak, our departmental member received a Prof. Vratislav Bedjanič Award for outstanding academic work in the field of industrial automation and electroenergetics for his diploma thesis entitled "The application of electrochemical impedance spectroscopy to PEM fuel cell systems".

the water conditions inside a PEM fuel-cell stack. This year an experimental study of the PEM-fuel-cell water-condition diagnostics performed with the Electrochemical Impedance Spectroscopy (EIS) on the fuel-cell system produced by Hydrogenics was started. As the EIS was primary developed for diagnosing single fuel-cells, we first adapted the method in such a way that it became suitable for diagnosing larger fuel-cell stacks. Next, we conducted a series of measurements and we showed that the adapted method is effective at diagnosing the two main faults occurring during the fuel-cell system operation - the drying of the PEM membranes and the flooding of the gas-diffusion layer (Figure 2).

The sub-area tools and building blocks for implementation also included three parts. The first part of our work was devoted to a further development of the program package for rapid prototyping of the advanced control algorithms. Control-systems-implementation environment is currently under integration with the program package "IDR blok" (a software package for the PLC controllers).

In the frame of the research dealing with the tools and methodologies for a process-control-software synthesis, the already-developed modeldriven engineering approach to industrial process-control software was extended and named MAGICS (Modelling and Automatic Generation of the Industrial Process-Control Software). MAGICS approach consists of two engineering levels, development activities and guidelines, the formalized ProcGraph language and a supporting tool suite. One of the supporting tools

has been newly developed - a professional version of the model editor (Figure 3).

In cooperation with the Center of Excellence for Low-Carbon Technologies (CONOT) we designed new components for the fuel-cell-based power systems. These include a controlled heater for the prevention of freezing of a stack, a prototype of a diagnostic module and a DC/DC converter (Figure 4). The DC/DC converter for the fuel-cell power systems is a conversion module converting the output voltage from the fuel-cell power module to the voltage of the energy-storage device. The control of the DC/DC converter is provided through the CAN-bus communication. Each converter is capable of a 2-kW power transfer and could be paralleled to obtain higher output currents. Each converter has a built-in stimulus generator intended for the support of the electrochemical impedance spectrometry of the fuel-cell stack during the operation.

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 way of obtaining a more uniform thickness of metal sheets in cold rolling is to reduce the variance in the control input. This can be done by feeding the controller with the de-noised signals. The de-noising approach based on the adaptive Kalman filter was proposed, resulting in a reduction of the high-frequency content of the signal while guarantying an asymptotic tracking of the "noise-free" component of the signal. The work has been carried out in the frame of the international project called PROBASENSOR.

A function block for the implementation of an explicit predictive controller on a programmable logic controller platform has been developed. This block enables the implementation of an MPC controller featuring advanced handling of the constraints on the process signals using standard industrial automation equipment.

The control of the wastewater-treatment plants is our traditional research area. In the area of the wastewater treatment a multi-criteria evaluation methodology for determining the optimum operating strategies for an

anaerobic-digestion reactor under uncertainty was proposed. The method is based on the Monte-Carlo simulations and the probability theory in order to deal with the analysis of choices among risky operation strategies with multi-dimensional outcomes.



Figure 3: Screenshot of the professional version of the ProcGraph model editor

The 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 the product quality with no obvious reasons.

Through the cooperation with the Kolektor Sinabit company a procedure for a systematic selection of the influential parameters in the pulley-production process has been developed. Additionally, we analysed their influence on the end-quality of the product. The information about these parameters is used to construct a mathematical model of the production process that can be used to reduce the possibility of faults and ensure a constant quality of the products.

In the field of production control, we continued with the evaluation of a hierarchical concept of a model-based production control. In the past year we reviewed this area and determined general instructions on implementing the Key Performance Indicators in the production; we also explored different methods for the input of a variable selection and determined controllability measures to examine the achievable output space.

In the recent years, a part of our work was focused on the area of fuel cells. In 2011 we became involved in two new EU 7FP projects: "Fuel Cell Based On-Board Power Generation (FCGEN)" and ""Fluid Management component improvement for Back up fuel cell systems (FluMaBack)". The objective of the FCGEN project is to develop and demonstrate an auxiliary Figure 4: DC/DC converter for fuel-cell power systems power unit (APU) for trucks that uses an auto-thermal reformer to produce

hydrogen from fuel and a fuel-cell stack for electricity production. The goal is to substitute the low-efficiency mainengine idling and provide for the electricity consumption. Within the project both the key components and the system design will be further developed. The role of our group is to develop the power conditioning, complete electronics

and to set up a control for all the subsystems and for the integrated APU system. In the FluMaBack project our group is responsible for improving the performance, the cost effictiveness and the life time of the essential balance-of-plant (BOP) components used in a fuel cell on the basis of the uninterruptable power back-up systems.

Within the multidisciplinary project "Integration and control of liquid fuel processor based on ceramic micro-systems (CERACON)" we continue

to develop the prototypes of the critical components of the miniature-sized fuel reformer that will serve as a source of hydrogen for the miniature fuel cells. The project is financed by the European Space Agency and performed in a collaboration of four partners: the Jozef Stefan Institute (Dept. of Electronic Ceramics and Dept. of Systems and Control), the National Institute of Chemistry, Slovenia (the Laboratory of the Catalysis and Chemical Reaction Engineering) and the company Hipot RR.

#### **R&D** projects for the industry and other users

A significant part of the development activities of our department is oriented towards the implementation of fuel cells in various applications and the development of special-purpose modules for fuel cells based on generator sets. The development related to the fuel-cell-based systems applications has been performed mostly within the Centre of Excellence for Low-Carbon Technologies where our group is leading these activities within the centre.

In 2011 we started with the activities within the Competence Centre for Advanced Control Technologies (CC ACT), which is co-financed by the Ministry of Higher Education, Science and Technology, and the European Regional Development Fund. In the competence centre, which involves 17 partners, we are actively involved in 6 out of 7 R&D projects addressing the design of the new components for the implementation of advanced control, the model-based production control, the control and optimization of the efficient energy consumption and clean environment, the automatic condition monitoring of the process equipment and the fusion power-plant control. This year we carried out an analysis of the project requirements and the design of the specifications for the new solutions, which will be implemented in collaboration with the key engineering companies involved in production automation and informatics: Danfoss, Helios and Litostroj Power.



The department acquired the project "Integration and control of liquid fuel processor based on ceramic microsystems" financed by the European Space Agency.



Figure 5: Electromotor during on-line diagnostics testing

The process-control tool C Batch, a partner product of INEA, d.o.o. and Mitsubishi Electric, whose principal developer is our departmental member Giovanni Godena, was chosen as the second best product of the month in the competition organised by a German magazine CAV. As described below, an important part of our activities is also devoted to direct cooperation with various companies.

In 2011 an important part of the activities 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 the recipe-based batch process-control packages for the PLC platform (PLCbatch, RTbatch, Cbatch), an automatic generation of the parts of the application code was realized to avoid entering the same information repeatedly into different parts of the control system. The record-

ing and archiving of the process events and the generating of the production reports were also implemented. In order to improve the commercialization of the tool, a professional user manual was written.

Within the "Kibernet" project that was, in 2011, completed in cooperation with the Inea company, a programme module for calculating the user reliability in the Microsoft Visual Basic.NET, in the form of a windows service, has been implemented. The service was incorporated into the integrated system of the service centre for electric-energy demand-side management.

In the framework of the ongoing project with Danfoss "intelligent" and integrating valve drives are being developed. In case of faults, soft sensors and optimization of actuators are applied.

The R&D group of Danfoss Trata d.o.o. and our Department of Systems and Control received the silver prize of the Chamber of Commerce and Industry of Slovenia for the HVAC electric valve innovation. At the Domel Company, Železniki, a new diagnostic system for endquality control on the production line for electrical motors of type 462 was completely installed in 2011 (Figures 5 and 6). The system is characterized by a new set of manipulators that enable suitable acoustical and vibrational isolation of the motors during the measurements on the production line. The new system is the fifth in the row of similar, very successful, diagnostic systems used in Domel. Up till now, the implemented systems have been pateral of more than 15 million motors.

used for the final-production quality control of more than 15 million motors. Within the review of the preliminary design of the third stage of the Ljubljana Waste Water Treatment Plant,

which was performed for the municipal company VO-KA in Ljubljana, a mathematical model of the existing plant



Figure 6: Diagnostic system for end-quality control on the production line for electrical motors of type 462 at Domel d.o.o.

Installation of an automatic diagnostic system for the total end-quality control of electrical motors on the production line ML-7 at Domel d.o.o. (Janko Petrovčič, Gregor Dolanc, Bojan Musizza, Stane Černe, Miroslav Štrubelj). was designed and upgraded with the proposed technical solutions for an improved nitrogen and phosphorus removal. Simulation tests were performed to verify the compliance of the upgraded plant performance with the legislation requirements.

### **Other projects**

In 2011 the activities within the project »Promoting Innovation in the Industrial Informatics and Embedded Systems Sector through Networking – I3E« funded by **\*the South East Europe-Transnational Cooperation Programme**« have been continued. The basic objectives of this project are the promotion of innovation and entrepreneurship in the area of Southeast Europe with an emphasis on the development of advanced products and services in the sectors of industrial informatics and embedded systems. This year our group has collaborated with the other partners in the completion of the main project outcome called the Strategic Research Agenda. We are also developing a Methodology Guideline for Innovation supporting the transformation of research into innovation. The main project outcomes are disseminated within several workshops to the relevant audience from the South-East Europe Region.

### Educational and training activities

Some members of the department give lectures and practical courses at different faculties and universities: the Faculty of Electrical Engineering, the University of Ljubljana, the Faculty of Logistics, the 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.

Special care was given to post-qualification training for the engineers from the industry. In 2011 topical courses covering the areas of control theory and its applications were organised for companies Danfoss and Cosylab.

### Some outstanding publications in the past year

- 1. Boštjan Pregelj, Darko Vrečko, Vladimir Jovan, Improving the operation of a fuel-cell power unit with supervision control - a simulation study. J. power sources, [Print ed.], 2011, vol. 196, no. 22, str. 9419-9428, 2011, doi:[COBISS.SI-ID 1016/j.jpowsour.2011.06.07724858151.]
- 2. Pavle Boškoski, Janko Petrovčič, Bojan Musizza, Đani Juričić, An end-quality assessment system for electronically commutated motors based 3 on evidential reasoning, Expert syst. appl., .. [Print ed.], 2011, vol. 38, no. 11, str. 13816-13826, 2011, doi:[COBISS.SI-ID 10.1016/j.eswa.2011.04.18524756775.]
- 3. Nadja Hvala, Fernando Aller, Teodora Miteva, Dolores Kukanja, Modelling, simulation and control of an industrial, semi-batch, emulsion-polymerization reactor«,. Comput. chem. eng., .. [Print ed.], 2011, vol. 35, no. 10, str. 2066-2080, 2011, doi: [COBISS.SI-ID 10.1016/j.compchemeng.2011.05.01624978727.]
- Matej Gašperin, IĆ, Đani Juričić, BOŠKOSKI, Pavle Boškoski, VIŽINTIN, Jože Vižintin,. Model-based prognostics 4. of gear health using stochastic dynamical models,. Mech. syst. signal process., 2011, vol. 25, no. 2, str. 537-548, 2011, doi:[COBISS.SI-ID 10.1016/j.ymssp.2010.07.00323786791.]

### Awards and appointments

- Andrej Debenjak: at the regional IEEE student competition during the ERK 2011 Conference won the competition 1. among seven contributions. His work addressed the application of electrochemical impedance spectroscopy to PEM fuel-cell systems.
- Andrej Debenjak: received a Prof. Dr. Vratislav Bedjanič Award for his diploma thesis entitled The application 2. of electrochemical impedance spectroscopy to PEM fuel cell systems.
- Dejan Petelin: appointment for design, organization and editing proceedings for the 3rd Student Conference 3. of the Jožef Stefan International Postgraduate School
- Damir Vrančić, JSI, Janko Petrovčič, JSI, Samo Krančan, Danfoss Trata: Silver and gold prizes for the HVAC 4. electrical valve innovation granted by the Chamber of Commerce and Industry of Slovenia

### INTERNATIONAL PROJECTS

- Fuel Cell Based On-board Power Generation FCGEN 7. FP 277844 EC; Jazaer Dawody, Volvo Technology Corporation, 06130 Exhaust Aftertreatment & Fuel Reforming, Göteborg, Sweden Dr. Boštjan Pregelj Probalistic Bayesian Soft Sensor - A Tool for On-line Estimation of the Key Process Variable in Cold Rolling Mills ProBaSensor EUROSTARS COMPUREG Plzen, s.r.o., Czech Republic Prof. Đani Juričić Promoting Innovation in the Industrial Informatics and Embedded Systems Sectors through Networking 13E South East Europe Programme SEE/A/219/1.1/X Dr. Athanasios Kalogeras, Industrial Systems Institute / Research Centre ATHENA, Patras, Greece Dr. Vladimir Iovan Integration and Control of Liquid Fuel Processor on Ceramic Micro-systems CERACON ESA PECS, 4000103742/11/NL/KML Bernard Zufferey, ESA - The European Space Agency, Paris, France; European Space Research and Technology Centre, Noordwijk, The Netherlands Dr. Gregor Dolanc, Asst. Prof. Marko Hrovat
- Intelligent Monitoring, Control, and Security of Critical Infrastructure Systems IntelliCIS COST IC0806

  - EC; COST Office, Brussels, Belgium Dr. Nadja Hvala
- Combining Soft Computing Techniques and Statistical Methods to Improve Data

Analysis Solutions SOFTSTAT COST IC0702 EC; COST Office, Brussels, Belgium Prof. Juš Kocijan

- Specification of the Automation System for the Metal Plate Treatment Machine Using Plasma B0-10-0009
  - Primož Eiselt, PlasmaBull Engineering GmbH, Lebring, Austria
- Dr. Gregor Dolanc System Identification Based on Gaussian Process Model for Traffic Control Applications BI-CZ/10-11-014 Dr. Jan Prikryl, Institute of Information Theory and Automation, Czech Academy of

Science, Prague, Czech Republic Prof. Juš Kocijan

# R & D GRANTS AND CONTRACTS

- Identification and model analysis for dynamic systems control design with Gaussian 1. process priors
- Prof. Juš Kocijan 2 Integrated diagnostic system for drive assemblies
- Prof. Đani Juričić
- 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 4 complex production processes Prof. Đani Juričić
- Simplified explicit predictive controller Prof. Stanislav Strmčnik

- Prognostics and health management of mechanical drives based on novel MEMS sensor networks Prof. Dani Juričić
- Feasibility study for setting up Technology Development Centre "Japanese hub" in Slovenia for technology fields of new energy tehnologies and process control technologies Prof. Stanislav Strmčnik

# RESEARCH PROGRAM

1. Program systems and control Prof. Dr. Đani Juričić

# NEW CONTRACTS

 Development activities on HyCore project-Development of key subsystems for high temperature PEM fuel cells Inea d. o. o. Dr. Vladimir Jovan

# MENTORING

### Ph. D. Theses

- Pavle Boškoski, Condition monitoring of mechanical drives: feature extraction and fault diagnosis methods (mentor Đani Juričić; co-mentor Mile Stankovski).
- Matej Gašperin, Parameter estimation of nonlinear dynamic systems with application to failure prognostics (mentor Đani Juričić).
- Satja Lumbar, Predictive control of aircrafts based on visual servoing (mentor Drago Matko; co-mentor Stanko Strmčnik).

### M. Sc. Theses

- Tadej Kodelja, Simulation of system dynamics models with Simulink software (mentor Juš Kocijan).
- Edvin Raubar, Increasing productivity of ship-to-shore cranes in Port of Koper using advanced electronic systems (mentor Damir Vrančić; co-mentor Dani Juričić).

### Bologna M. Sc. Theses

 Staša Györköš, An introduction of the new approach to the designing of continuous model for the purpose of stochastic inventory control (mentor Damir Vrančić; comentor Dejan Dragan).

- Prognostics and health management of mechanical drives based on novel MEMS sensor networks Domel d o o
  - Prof. Đani Juričić
- Support for the research programme of Aleksander Preglej in the area of advanced control algorithms Inea d. o. o.
- Dr. Samo Gerkšič
- Upgrade and development of AMV 435 and AMV 65X valve drives Danfoss Trata, d. o. o. Asst. Prof. Damir Vrančić
- Functional upgrades of diagnostic systems Domel, d.o.o. Dr. Janko Petrovčič
- 2. Marko Intihar, Path planing in the process of acquistion of biological samples in the General hospital Celje (mentor Đani Juričić; co-mentor Dejan Dragan).
- Grega Medved, The development of sophisticated inventory management policies with variable demand accompanied with a comparative analysis of obtained results (mentor Damir Vrančić; co-mentor Dejan Dragan).
- Tea Vizinger, Development of the heuristic algorithm in the process of the biological material acquisition scheduling (mentor Đani Juričić; co-mentor Dejan Dragan).

# VISITORS FROM ABROAD

- 1. Dr. Ilaria Rosso, Electro Power Systems SpA, Torino, Italy, 9 June 2011
- Dr. Miroslav Kárný, Institute of Information Theory and Automation, Czech Academy of Sciences, Prague, Czech Republic, 19–21 June 2011
- Dr. Jan Přikryl, Institute of Information Theory and Automation, Czech Academy of Sciences, Prague, Czech Republic, 24 August to 27 September 2011
- 4. Luka Cetina, Novatec d.o.o., Labin, Croatia, 16 September 2011
- 5. Roberto Gobo, Novatec d.o.o., Labin, Croatia, 16 September 2011
- 6. Damir Ratković, Novatec d.o.o., Labin, Croatia, 16 September 2011
- David DeVries, Genesis Fueltech Inc., Spokane Valley, USA, 18-19 September 2011
   Dr. Ladislav Jirsa, Institute of Information Theory and Automation, Czech Academy
- Dr. Ladislav Jirsa, Institute of Information Theory and Automation, Czech Academy of Sciences, Prague, Czech Republic, 21–24 September 2011
- Dr. Kamil Dedecius, Institute of Information Theory and Automation, Czech Academy of Sciences, Prague, Czech Republic, 21–24 September 2011

# STAFF

### Researchers

- 1. Dr. Gregor Dolance
- 2. Dr. Samo Gerkšič
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   Dr. Nadja Hvala
- 6. Dr. Vladimir Jovan, Head
- 7. Prof. Đani Iuričić
- 8. Dr. Gregor Kandare
- 9. Prof. Juš Kocijan
- 10. Dr. Janko Petrovčič
- Prof. Stanislav Strmčnik
   Asst. Prof. Damir Vrančić
- ASSI, PTOI, Damir Vrančić
   Dr Darko Vrečko

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- 14. Dr. Matej Gašperin
- 15. Dr. Bojan Musizza

16. Dr. Marko Nerat 17. Dr. Boštjan Pregelj Postgraduates 18. Dr. Pavle Boškoski 19. Andrej Debenjak, B. Sc. 20. Miha Glavan, B. Sc. 21. Tomaž Lukman, B. Sc. 22. Dr. Satja Lumbar, left 01.07.11 23. Jernej Mrovlje, M. Sc. 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** 28. Maja Janežič, B. Sc. 29. Miroslav Štrubelj

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- 3. Pavle Boškoski, Janko Petrovčič, Bojan Musizza, Đani Juričić, Andrej Biček, "End-quality assessment of electrical motors based on the concept of virtual sensors", *Ventil (Ljubl.)*, vol. 17, no. 2, pp. 148-153, 2011.
- 4. Pavle Boškoski, Anton Urevc, "Bearing fault detection with application to PHM data challenge", *Int. j. progn. health manag.*, vol. 2, no. 1, pp. 003-1-003-10, 2011.
- Aljaž Čufar, Vladimir Jovan, "Ocena bilance vode v sistemu reformer/gorivne celice", *Elektrotehniški vestnik*, vol. 78, no. 1/2, pp. 61-66, 2011.
- Dejan Dovžan, Vito Logar, Nadja Hvala, Igor Škrjanc, "Monitoring and sensor fault detection in a waste-water treatment process based on a fuzzy model", *Elektrotehniški vestnik*, vol. 78, no. 3, pp. 142-146, 2011.
- Dejan Dovžan, Vito Logar, Nadja Hvala, Igor Škrjanc, "Zaznavanje napak in spremljanje čiščenja odpadnih voda na podlagi mehkega modela", *Elektrotehniški vestnik*, vol. 78, no. 3, pp. 142-146, 2011.
- 8. Andrej Fabjan, Bojan Musizza, Fajko Bajrović, Marjan Zaletel, Martin Štrucl, "The effect of the cold pressor test on a visually evoked cerebral blood flow velocity response", *Ultrasound med. biol.*, Nov 18, 2011.
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- 11. Dejan Gradišar, "Interreg IV projekt I3E: pospeševanje inovacij na področjih industrijske informatike in vgrajenih sistemov z medsebojnim povezovanjem", *Ventil (Ljubl.)*, vol. 17, no. 4, pp. 308-309, 2011.
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- 15. Gregor Kandare, Antonio Nevado Reviriego, "Adaptive predictive expert control of dissolved oxygen concentration in a wastewater treatment plant", *Water sci. technol.*, vol. 64, no. 5, pp. 1130-1136, 2011.
- 16. Juš Kocijan, Dejan Petelin, "Output-error model training for Gaussian process models", In: Adaptive and natural computing algorithms: 10th international conference, ICANNGA 2011, Ljubljana, Slovenia, April 14-16, 2011: proceedings, *Lect. notes comput. sci.*, vol. 6594, pp. 312-320, 2011.
- 17. Tomaž Lukman, Raymond A. Hackney, Aleš Popovič, Jurij Jaklič, Zahir Irani, "Business intelligence maturity: the economic transitional context within Slovenia", *Inf. syst. manage.*, vol. 28, iss. 3, pp. 211-222, Summer 2011.
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- Dejan Petelin, Juš Kocijan, Alexandra Grancharova, "On-line Gaussian process model for the prediction of the ozone concentration in the air", *Dokl. B"Ig. akad. nauk.*, vol. 64, no. 1, pp. 117-124, 2011.
- Boštjan Pregelj, Samo Gerkšič, "Hybrid explicit model predictive control of a nonlinear process approximated with a piecewise affine model", *J. process control*, vol. 20, no. 7, pp. 832-839, 2011.
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- 24. Darko Vrečko, Nadja Hvala, Marjeta Stražar, "The application of model predictive control of ammonia nitrogen in an activated sludge process", *Water sci. technol.*, vol. 64, no. 5, pp. 1115-1121, 2011.

### PUBLISHED CONFERENCE PAPERS

### **Invited Papers**

- 1. Darko Belavič, Marko Hrovat, Gregor Dolanc, Janez Holc, Marina Santo-Zarnik, Primož Fajdiga, Kostja Makarovič, Stanko Hočevar, Jurka Batista, Iztok Stegel, "A chemical microreactor as an example of an LTCC-based ceramic microsystem", In: *Proceedings*, Electronic Devices and Systems, [EDS'11] IMAPS CS International Conference, June 22-23, 2011, Brno, Czech Republic, Ondrej Hegr, ed., Brno, Vysoké učeni technické, 2011, pp. XIII-XVIII.
- 2. Đani Juričić, Pavle Boškoski, Matej Gašperin, "Advances in diagnostics and prognostics of mechanical drives", In: *Proceedings of COSY 2011 papers: in honour of professor Georgi M. Dimirovski*, Special International Conference on Complex systems: synergy of control communications and computing, September 16-20, 2011, Ohrid, Republic of Macedonia, Tatjana Kolemishevska-Gugulovska, ed., Mile J. Stankovski, ed., Skopje, Society for Electronics, Telecommunications, Automation, and Informatics of the Republic of Macedonia, 2011, pp. 287-296.
- 3. Juš Kocijan, "Control algorithms based of Gaussian process models: a state-of-the-art survey", In: *Proceedings of COSY 2011 papers: in honour of professor Georgi M. Dimirovski*, Special International Conference on Complex systems: synergy of control communications and computing, September 16-20, 2011, Ohrid, Republic of Macedonia, Tatjana Kolemishevska-Gugulovska, ed., Mile J. Stankovski, ed., Skopje, Society for Electronics, Telecommunications, Automation, and Informatics of the Republic of Macedonia, 2011, pp. 69-80.

### **Regular** papers

- 1. Darko Belavič, Marko Hrovat, Gregor Dolanc, Stanko Hočevar, Iztok Stegel, Marina Santo-Zarnik, Janez Holc, Kostja Makarovič, Jurka Batista, Primož Fajdiga, Marija Kosec, "Design and fabrication of a complex LTCC-based reactor for the production of hydrogen for portable PEM fuel cells", In: *Proceedings*, 2011 IMAPS/ACerS, 7th International Conference and Exhibition on Ceramic Interconnect and Ceramic Microsystems Technologies (CICMT), April 5-7, 2011, San Diego, California, USA, Washington, International Microelectronics and Packaging Society, 2011, pp. 23-28.
- Darko Belavič, Marina Santo-Zarnik, Marko Hrovat, Janez Holc, Kostja Makarovič, Gregor Dolanc, "Thermal design of LTCC based ceramic microsystem", In: *Proceedings*, 35th International Microelectronics and Packaging IMAPS - IEEE CPMT Poland Conference, September 21-24, 2011, Gdańsk-Sobieszevo, Piotr Jasiński, ed., Grzegorz Jasiński, ed., [S. l.], IMAPS-CPMT, 2011, pp. 89-92.
   Pavle Boškoski, Đani Juričić, "Point processes for bearing fault
- 3. Pavle Boškoski, Đani Juričić, "Point processes for bearing fault detection under non-stationary operating conditions", In: *PHM*`11: proceedings of The Annual Conference of the Prognostics and Health Management Society 2011, September 25-29, 2011, Montreal, Quebec, Canada, [S. l.], PHM Society, 2011, pp. 427-434.
- 4. Jani Čebokli, Andrej Debenjak, "Vrednotenje učinkovitosti različnih metod načrtovanja vodenja orientacije satelita", In: Zbornik sedme konference AlG'11 Avtomatizacija v industriji in gospodarstvu, 31. marec in 1. april 2011, Maribor, Slovenija, Boris Tovornik, ed., Nenad

Muškinja, ed., Milan Rotovnik, ed., [Maribor], Društvo avtomatikov Slovenije, [2011], pp. 1-6.

- Andrej Debenjak, "Uporaba elektrokemične impedančne spektroskopije v sistemih s PEM gorivnimi celicami", In: Zbornik dvajsete mednarodne Elektrotehniške in računalniške konference ERK 2011, 19.-21. september 2011, Portorož, Slovenija, (Zbornik ... Elektrotehniške in računalniške konference ERK ...), Baldomir Zajc, ed., Andrej Trost, ed., Ljubljana, IEEE Region 8, Slovenska sekcija IEEE, 2011, zv. B, pp. 467-468.
- 6. Matej Gašperin, Pavle Boškoski, Đani Juričić, "Diagnostična in prognostična platforma za avtomatsko spremljanje stanja opreme", In: *Vir znanja in izkušenj za stroko: zbornik foruma*, Industrijski forum IRT, Portorož, 6. in 7. junij 2011, Tomaž Perme, ed., Darko Švetak, ed., Škofljica, Profidtp, 2011, pp. 103-108.
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- 10. Miha Glavan, Dejan Gradišar, "Modeliranje z nevronskimi mrežami za namene vodenja proizvodnje", In: *Zbornik sedme konference AIG'11 Avtomatizacija v industriji in gospodarstvu, 31. marec in 1. april 2011, Maribor, Slovenija*, Boris Tovornik, ed., Nenad Muškinja, ed., Milan Rotovnik, ed., [Maribor], Društvo avtomatikov Slovenije, [2011], 7 pp.
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- 12. Dejan Gradišar, Vladimir Jovan, "Predstavitev strateške raziskovalne usmeritve I3E", In: Zbornik sedme konference AIG'11 Avtomatizacija v industriji in gospodarstvu, 31. marec in 1. april 2011, Maribor, Slovenija, Boris Tovornik, ed., Nenad Muškinja, ed., Milan Rotovnik, ed., [Maribor], Društvo avtomatikov Slovenije, [2011], 7 pp.
- 13. Alexandra Grancharova, Juš Kocijan, "Explicit stochastic model predictive control of gas-liquid separator based on Gaussian process model", In: *Proceedings: John Atanasoff celebration days*, International Conference Automatics and Informatics '11, Bulgaria, Sofia, October 3-7, 2011, Sofia, John Atanasoff Society of Union of Automation and Informatics, 2011, pp. B-85-B-88.
- 14. Marko Hrovat, Darko Belavič, Gregor Dolanc, Janez Holc, Marina Santo-Zarnik, Primož Fajdiga, Kostja Makarovič, Marija Kosec, Stanko Hočevar, Jurka Batista, Iztok Stegel, "The LTCC combustor for ceramic micro-reactor for steam reforming", In: *New trends in micro/nanotechnology*, ISSE 2011, 34th International Spring Seminar on Electronics Technology, May 11-15, 2011, High Tatras, Slovakia, Alena Pietrikóva, ed., Manuela Franz, ed., Johann Nicolics, ed., Košice, Technical University of Košice, Faculty of Electrical Engineering and Informatics, 2011, 4 pp.
- 15. Ulf Jeppsson it et. al. (17 authors), "Quo vadis benchmark simulation models?", In: *Conference proceedings*, 8th International IWA Symposium on Systems Analysis and Integrated Assessment, WATERMATEX 2011, 19-22 June 2011, San Sebastian, Spain, [S. l.], International Water Association, 2011, pp. 493-506.
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- 17. Đani Juričić, Pavel Ettler, Juš Kocijan, "Fault detection based on Gaussian process models: an application to the rolling mill", In: *Proceedings. Volume 2*, ICINCO 2011, 8th International Conference on Informatics in Control, Automation, 28-31 July 2011,

Noordwijkerhout, The Netherlands, Jean-Louis Ferrier, ed., [S. l.], SciTePress, = Science and Technology Publications, 2011, pp. 437-440.

- 18. Gregor Kandare, Mitja Bizjak, "Sistem za pametno krmiljenje industrijskih bremen in razpršene proizvodnje električne energije", In: Zbornik sedme konference AIG'11 Avtomatizacija v industriji in gospodarstvu, 31. marec in 1. april 2011, Maribor, Slovenija, Boris Tovornik, ed., Nenad Muškinja, ed., Milan Rotovnik, ed., [Maribor], Društvo avtomatikov Slovenije, [2011], 6 pp.
- 19. Juš Kocijan, Vesna Tanko, "Prognosis of gear health using Gauissian process model", In: *EUROCON 2011*, International Conference on Computer as a Tool, April, 27., 28., 29. 2011, Lisbon, Portugal, [S. l., s. n.], 2011, 4 pp.
- 20. Jernej Mrovlje, Edvin Raubar, Damir Vrančić, "Samodejno določanje položaja vlačilcev s pomočjo stereoskopije", In: *Vir znanja in izkušenj za stroko: zbornik foruma*, Industrijski forum IRT, Portorož, 6. in 7. junij 2011, Tomaž Perme, ed., Darko Švetak, ed., Škofljica, Profidtp, 2011, pp. 76-70.
- 21. Dejan Petelin, Juš Kocijan, "Control system with evolving Gaussian process models", In: *Proceedings*, (IEEE Symposium series on computional inteligence), EAIS 2011, 2011 IEEE Workshop on Evolving and Adaptive Intelligent Systems, April 11-15, 2011, Paris, France, Piscataway, IEEE, 2011, pp. 178-184.
- 22. Dejan Petelin, Jan Šindelář, Jan Příkryl, Juš Kocijan, "Financial modeling using Gaussian process models", In: *IDAACS'11: proceedings* of the 6th IEEE International Conference on Intelligent Data Acquisition and Advanced Computing Systems: Technology and Applications, 15-17 September, 2011, Prague, Czech Republic. 2 Vol., Piscataway, IEEE, = Institute of Electrical and Electronics Engineers, cop. 2011, vol. 1, pp. 672-677.
- 23. Boštjan Pregelj, Darko Vrečko, Vladimir Jovan, "Vodenje hibridnega agregata z gorivnimi celicami", In: *Zbornik sedme konference AlG'11 Avtomatizacija v industriji in gospodarstvu, 31. marec in 1. april 2011, Maribor, Slovenija*, Boris Tovornik, ed., Nenad Muškinja, ed., Milan Rotovnik, ed., [Maribor], Društvo avtomatikov Slovenije, [2011], 7 pp.
- 24. Damir Vrančić, "Design of MIMO Controllers with inverted decoupling", In: *Final program and proceedings*, (Besedilni podatki), ASCC 2011, The Eighth Asian Control Conference, May 15-18, 2011, Kaohsiung, Taiwan, Wonmi-gu, Asian Control Association, cop. 2011, pp. 1153-1158.
- Damir Vrančić, Mikuláš Huba, "Design of feedback control for unstable processes with time delay", In: *Proceedings*, 18th International Conference on Process Control, June 14-17, 2011, Tatranská Lomnica, Slovakia, Bratislava, Institute of Information Engineering, Automation and Mathematics, 2011, pp. 100-105.
   Damir Vrančić, Stanko Strmčnik, "Design of 2-DOF PI controller for
- 26. Damir Vrančić, Stanko Strmčnik, "Design of 2-DOF PI controller for integrating processes", In: *Final program and proceedings*, (Besedilni podatki), ASCC 2011, The Eighth Asian Control Conference, May 15-18, 2011, Kaohsiung, Taiwan, Wonmi-gu, Asian Control Association, cop. 2011, pp. 1135-1140.
- 27. Darko Vrečko, Nadja Hvala, Marjeta Stražar, "Modelling and simulation to improve the operation of the sludge treatment process", In: *Conference proceedings*, 8th International IWA Symposium on Systems Analysis and Integrated Assessment, WATERMATEX 2011, 19-22 June 2011, San Sebastian, Spain, [S. l.], International Water Association, 2011, pp. 632-738.

### THESES

### Ph. D. Theses

- 1. Pavle Boškoski, *Condition monitoring of mechanical drives: feature extraction and fault diagnosis methods:* doctoral dissertation, Ljubljana, [P. Boškoski], 2011.
- Matej Gašperin, Parameter estimation of nonlinear dynamic systems with application to failure prognostics: doctoral dissertation, Ljubljana, [M. Gašperin], 2011.
- 3. Satja Lumbar, *Predictive control of aircrafts based on visual servoing:* doctoral dissertation, Ljubljana, [S. Lumbar], 2011.

### B. Sc. Thesis

1. Andrej Debenjak, *Electrochemical impedance spectroscopy usage in PEM fuel cell systems:* undergraduate thesis, Ljubljana, [A. Debenjak], 2011.

# ARTIFICIAL INTELLIGENCE LABORATORY

The Artificial Intelligence Laboratory is concerned mainly with the 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 realtime 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 a 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; AnswerArt (http://answerart.net/), a system for semantic search on large databases (AFSA, OpenCyc, WordNet); Enrycher (http://enrycher. ijs.si/), a system for the semantic enrichment of textual data; SearchPoint (http://searchpoint.ijs. si/), a portal for visual and contextualized Web browsing; Contextify (http://contextify.net/), a Prof. Dunja Mladenić tool for contextualized e-mail and contact management. The laboratory's strategy is to combine scientific excellence and strong collaboration with industry, and to transfer research results into real-world business environments.



Head:

In the last 10 years, members of the Artificial Intelligence Laboratory successfully completed 23 EU projects, of which 4 were concluded in 2011. In addition, we were involved in another 11 EU 7FP projects in 2011, including three 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 the beginning of 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, focused on developing the methods for dealing with high-dimensional data while taking the hubness phenomenon into account: we proposed new supervised learning methods (best paper award at the MLDM-2011 international conference) and new unsupervised learning methods (second-best paper award at the PAKDD-2011 international conference). We extended

the existing statistical methods for analyzing multiple-source data (e.g., text documents in several natural languages) to support the use of a larger number of data sources. Within our collaboration in the bilateral project with Serbia called Linking images and text: expanding image analysis with machine learning and semantic technologies, we constructed a database of tagged images from the publicly available Wikipedia data and processed it with the machine learning methods for simultaneous handling of images and the accompanying text. Within the ESC (European Security Challenge) EU project, we defined the rules and guidelines for organizing competitions dealing with the security of machine-learning-based technologies.

Our work on text and network analysis connects the language technologies, machine learning, semantic technologies and cross-modal data processing methods. Our activities included the development of new word sense disambiguation methods using multiple ontologies taken from the Linked Open Data initiative. Within ALERT (active support and real-time coordination based on event processing in FLOSS development), an EU 7FP project, we expanded our text-mining methods to cover the analysis of the software source code, where a combined analysis of a source code and discussions from a bug-tracking system can improve the debugging efforts in the open-source software development. Within Planet Data (Intelligent In 2011 we started participating in two centres of excellence and the related new applied projects, as well as continuing our ongoing collaboration in 15 EU projects.



Figure 1: Semantic Knowledge Management: Integrating Ontology Management, Knowledge Discovery, and Human Language Technologies, edited by J. Davies, M. Grobelnik and D. Mladenić; published by Springer. This book describes approaches and methods for the integration of ontology management, data mining and language technologies.

In 2011 we won the best paper award at the International Conference on Machine Learning and Data Mining, the second-best paper award at the Pacific-Asia Conference on Knowledge Discovery and Data Mining, and the third-best demo award at the Extended Semantic Web Conference. *Information Management)*, an EU network of excellence, we developed a system for studying a corpus of semantically enriched texts through time, as well as developing the methods for a semantic enrichment of sensor networks. In collaboration with the Institute's Communication Systems Department (E6) we incorporated these methods into the VIDEK demo application, which enables intelligent monitoring of the environmental sensor data (prize for the third-best demo at the ESWC-2011 international conference). We also developed a demo system for semantic search in sensor networks using the Personalized PageRank method. In the national project

called Slovenian Science Atlas we developed a system for search and visualization of research collaboration and competences of the scientists working in Slovenia. In *RENDER (Reflecting Knowledge Diversity)*, an EU 7FP project, we developed the methods to enrich the documents from social as well as traditional media with the goal of detecting the diversity of opinions in these sources. We concluded *VIDI (Visualising the Impact of the Legisla-*



Figure 2: Integrated analytic environment for anomaly detection, trend detection, route prediction and optimization, developed within the EURIDICE EU project.

*tion )*, an EU 7FP project, which improves the transparency of online forums and enables the discussions of both moderators and visitors.

In the area of **language technologies**, our activities in *METANet (Net Technologies for the Multilingual European Information Society)*, an EU network of excellence, were focused on the development and implementation of the efficient methods for automatic construction of multilingual corpora. Within *MultilingualWeb (Advancing the Multilingual Web)*, an EU 7FP project, we worked on the standards for, and concrete examples of, tools that support the construction, localization and use of multilingual web data. We also participated in the organization of the events that encourage the standardization of multilinguality on the web. Our current work concentrates on the named entity extraction. Within *Communication in Slovene*, a national project, we contributed to the development of the morphosyntactically tagged corpora and of automatic tagging methods.

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 ACTIVE (Enabling the Knowledge Powered Enterprise, an EU 7FP project, in which we developed the methods for modelling informal processes in large organizations, as well as the methods for modelling a context with the goal of predicting the information source usage. Together with the project partners we incorporated these methods into the Active Knowledge Workspace platform. We also developed Cycretary, an application that uses logical inference to simplify personal data management and personal schedule coordination. Our work within ENVISION (ENVIronmental Services Infrastructure with ONtologies) focused on the analysis of stream data and development of the methods for semantic enrichment of the sensor data. We also worked on search, clustering and personalization methods for partially-ordered data (e.g., SPARQL query results in semantic data bases). In the bilateral project with Romanian partners, Understanding human behaviour with an application to video

*surveillance,* we developed algorithms for semantic understanding of human behaviour in traffic from the video recordings and adapted hubness-based classification methods to detect objects in images. We also extended the existing publicly-available OntoGen system for a textual data visualization and ontology construction, enabling it

- Janez Brank won an award for his current work in the area of information society at the IS-2011 Conference
- Marko Grobelnik held invited talks at the Web Intelligence, Mining and Semantics Conference, as well as at the Korean Semantic Technology Conference

to process images in addition to texts and social network data.

In the area of knowledge management we successfully concluded *COIN* (*COllaboration and INteroperability for networked enterprises*), another 7FP project, covering the field of networked organizations, models and tools to support interoperability and inter-organizational collaboration. Within this project we developed applications supporting knowledge and competence modelling for groups of experts. We also concluded our work on the *EURIDICE (European Inter-Disciplinary Research on Intelligent Cargo*)

*for Efficient, Safe and Environment-friendly Logistics*) 7FP project, within which we developed and integrated an intelligent system for the control and management of container transport, as well as developing services for anomaly detection, trend detection, route prediction and optimization, knowledge discovery and formalization methods.

The Artificial Intelligence Laboratory puts special emphasis on the promotion of science. Part of our involvement in the national project called Youth Network of Research Values (SM-RIS) was the organization of a touring exhibition about the female PhD holders 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/). Within GENDERA (Gender Debate in the European Research Area), an EU 7FP project, we contributed to the establishment of an international best-practice database for the promotion of gender equality in research organizations; we also organized a national workshop on the same subject (http://ct3.ijs.si/gendera\_workshop\_2011/). Our work within SIS-Catalyst (Children as Change Agents for Science in Society), a 7FP project, was focused on the identification and collection of relevant data regarding the participation of young people at scientific events, exhibitions, workshops and summer schools that specifically target the youth. We started work on a new EU 7FP project, TransLectures (Transcription and Translation of Video Lectures), where we collaborate with the Centre for Knowledge Transfer in Information Technologies (CT3) on the automated subtitling and translating of video recordings. Together with CT3 we continued to use the videolectures. NET portal to promote artificial intelligence, the Institute, and the Slovenian research in general. Our laboratory is also the main organizer and supporter of the annual national ACM Computer Science Competition for secondaryschool students; this year, 309 students participated in the competition.

In 2011 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 three new projects, and being also appointed as coordinators of one of the largest projects. We continue with our successful efforts to include the Slovenian industry into the European research area; the list of 14 companies participating in EU projects has been extended by two. In total, we invited 6 Slovenian businesses to participate with us in the EU project proposals submitted in 2011.

### Some outstanding publications in the past year

- Inna Novalija, Dunja Mladenić, Luka Bradeško. OntoPlus: text-driven ontology extension using ontology content, structure and co-occurrence information. Knowl.-based syst. [Print ed.], 2011, vol. 24, no. 8, pp. 1261-1276, doi: 10.1016/j.knosys.2011.06.002.
- Nenad Tomašev, Miloš Radovanović, Dunja Mladenić, Mirjana Ivanović. Hubness-based fuzzy measures for high-dimensional k-nearest neighbour classification. Lect. Notes Comput. Sci., 2011, vol. 6871, pp. 16-30.
- Dunja Mladenić, Janez Brank, Marko Grobelnik. Document classification. In: Sammut, Webb, (eds.). Encyclopedia of machine learning: with 293 figures and 78 tables. New York: Springer, 2011, pp. 289-293.
- 4. Vadim Ermolayev, Frank Dengler, Carolina Fortuna, Tadej Štajner, Tom Bösser, Elke-Maria Melchior. Increasing predictability and sharing tacit knowledge in electronic design. In: Warren, Davies, Simperl (eds.). Context and semantics for knowledge management: technologies for personal productivity. Heidelberg: Springer, 2011, pp. 189-212.
- Polona Domadenik, Marko Grobelnik, Luka Pataky, Janez Prašnikar. Politically connected supervisory board members in Slovenian firms. In: Prašnikar (ed.). Slovenian economy stranded in recovery. 1st printing. Ljubljana: Časnik Finance, 2011, pp. 91-107.
   John Shawe-Taylor was the NIPS-2011 Conference; N

### Awards and appointments

1. Msc. Janez Brank: Award for the current achievements in the Information Society area



Figure 3: Work context detection system, developed within the ACTIVE EU project. When a user accesses an information source that is associated with a particular context, e.g., a web site or a textual document (in this case the contents of the web page lead to the detection of the context as being "Artificial Intelligence"), the system adapts to this context and can recommend other related information sources.

### Dunja Mladenić was a guest lecturer at the Cognitive Science Institute at the University of Quebec



Figure 4: One of the web forum visualizations, developed for the VIDI EU project. The application automatically detects the main topics of discussion and shows a chart of their importance through time (more relevant topics are indicated with thicker stripes). For example: the topic of nuclear energy (lower stripe) was highly relevant, but only for a short period in February.

John Shawe-Taylor was the general chair of the NIPS-2011 Conference; Marko Grobelnik was the programme committee chair of the Extended Semantic Web Conference

- 2. Dr. Blaž Fortuna, Carolina Fortuna, Marko Grobelnik, Klemen Kenda: Best demo award, ESWC 2011 conference, Crete, Greece
- 3. Prof. Mirjana Ivanović, prof. Dunja Mladenić, dr. Miloš Radovanović, Nenad Tomašev: Best paper award, MLDM 2011 conference, Newark, USA
- 4. Prof. Mirjana Ivanović, prof. Dunja Mladenić, dr. Miloš Radovanović, Nenad Tomašev: Best research paper runner up award, PAKDD 2011 conference, Shenzhen, China

### Organization of conferences, congress and meetings

- 1. Project meeting ALERT, Bled, 11–12 April 2011
- 2. Project meeting RENDER, Ljubljana, 19–20 April 2011
- 3. WWW 2011 conference, The 4th Semantic Search Workshop SemSearch'11, Hyderabad, India, 28 March to 1 April 2011
- 4. ESWC 2011 conference, tutorial The Web of Things, Heraklion, Crete, Greece, 29 May to 2 June 2011
- 5. ESWC 2011 conference, tutorial Semantic Technologies for Real-Time Data Processing, Heraklion, Crete, Greece, 29 May to 2 June 2011
- 14. International multiconference INFORMATION SOCIETY IS 2011, Conference on Data Mining and Data Warehouses – SIKDD 2011, 10–14 October 2011
- CIKM 2011 conference, workshop Search and Mining Entity-Relationship Data SMER'11, Glasgow, United Kingdom, 24–28 October 2011
- 8. GENDERA Slovenian National Workshop, Ljubljana, 12 December 2011

# INTERNATIONAL PROJECTS

1.	Transcription and Translation of Video Lectures		Technologiai Alapitvany, Budapest, Hungary
	transLectures		Prof. Dunja Mladenić, Mitja Jermol, M. Sc.
	7. FP, 287755	10.	Enabling the Knowledge Powered Enterprise
	EC; Alfons Juan, Universitat Politenica de Valencia, Valencia, Spain		ACTIVE
	Prof. Dunja Mladenič, Marko Grobelnik, Mitja Jermol, M. Sc.		7. FP, 215040
2.	Children as Change Agents for the Future of Science in Society		EC; Dr. Paul Warren, British Telecommunications plc, London, Great Britain
	SIS CATALYST		Marko Grobelnik, Prof. Dunja Mladenić, Mitja Jermol, M. Sc., Asst. Prof. Mihael
	7. FP, 266634		Mohorčič
	EC; The University of Liverpool, Liverpool, Great Britain	11.	Pattern Analysis, Statistical Modelling and Computational Learning 2
	Prof. Dunja Mladenić		PASCAL 2
3.	European Security Challenge		7. FP, 216886
	ESC		EC; Prof. John Shawe-Taylor, University of Southampton, Highfield, Southampton,
	7. FP, 261566		Great Britain
	EC; Simon Schneider, Global Security Challenge, London, Great Britain		Prof. Dunja Mladenić, Marko Grobelnik, Mitja Jermol, M. Sc.
	Marko Grobelnik, Prof. Dunja Mladenić	12.	European Inter-Disciplinary Research on Intelligent Cargo for Efficient, Safe and
4.	Active Support and Real-time Coordination based on Event Processing in Open Source		Environment-friendly Logistics
	Software Development		EURIDICE
	ALERT		7. FP, 216271
	7. FP, 258098		EC; Dr. Paolo Paganelli, INSIEL - Informatica per il Sistema degli Enti Locali s.p.a,
	EC; Dr. Ljiljana Stojanovic, Forschungszentrum Informatik an der Universität		Trieste, Italy
	Karlsruhe, Karlsruhe, Germany		Marko Grobelnik, Prof. Dunja Mladenić, Mitja Jermol, M. Sc., Dr. Špela Stres
	Prof. Dunja Mladenić, Marko Grobelnik, Mitja Jermol, M. Sc.	13.	Collaboration and INteroperability for networked enterprises
5.	PlanetData		COIN
	PlanetData		7. FP, 216256
	7. FP, 257641		EC; Dr. Claudia Guglielmina, TXT e-Solutions Spa, Milano, Italy
	EC; Alice Carpentier, Dieter Fensel, Universitaet Innsbruck, Innsbruck, Austria		Prof. Dunja Mladenić, Marko Grobelnik, Mitja Jermol, M. Sc.
	Marko Grobelnik, Prof. Dunja Mladenić, Mitja Jermol, M. Sc., Asst. Prof. Mihael	14.	Advancing the Multilingual Web
	Mohorčič		MultilingualWeb
6.	Reflecting Knowledge Diversity		CIP - Competitiveness and Innovation
	RENDER		250500
	7. FP, 257790		EC; Jérôme Chailloux, Caroline Baron, Celine Bitoune, GEIE ERCIM, Sofhia Antipolis,
	EC; Hartmut Schmeck, Karlsruhe Institute of Technology, Karlsruhe, Germany		France
	Prof. Dunja Mladenić, Marko Grobelnik, Mitja Jermol, M. Sc., Dr. Špela Stres		Marko Grobelnik, Prof. Dunja Mladenić
7.	Technologies for the Multilingual European Information Society MetaNet	15.	Communication in Slovenian Language
	7. FP, 249119		MŠŠ
	EC; Dr. Stefhan Busemann, DFKI - German Research Center for Artificial Intelligence,		Amebis d.o.o., Kamnik, Slovenija
	Saarbrücken, Germany	,	Dr. Simon Krek
	Marko Grobelnik, Prof. Dunja Mladenić, Mitja Jermol, M. Sc.	16.	Network of Research Values Development in Youth
8.	Environmental Services Infrastructures with Ontologies		SIM-RIS
	ENVISION		Prof. Dunja Mladenić
	7. FP, 249120	17.	Understanding Human Behavior for Video Surveillance Applications
	EC; Bjorn Skjellaug, Arne J. Berre, Stiftelsen Sintef, Trondheiim, Norway		BI-RO/10-11-010
	Prof. Dunja Mladenić, Miha Grčar, B. Sc., Prof. Nada Lavrač, Mitja Jermol, M. Sc.		Dr. Maria Magdalena Zaharescu, Ilie Murgulescu Institute of Physical Chemistry,
9.	Gender Debate in the European Research Area		Bucharest, Komania
	GENDERA	10	Prot. Dunja Mladenić
	/. fr, 244499	18.	Correlating Images and Words: Enhancing Image Analysis through Machine Learning
	EC; Dr. Dora Groo, Hungarian Science and Technology Foundation, Tudomanyos Es		and Semantic Technologies
			BI-5K/ 10-11-029

Dr. Mirjana Ivanović, Faculty of Science, Department of Mathematics and Informatics, Novi Sad Serbia Prof. Dunja Mladenić

# **R &D GRANTS AND CONTRACTS**

- 1. Information-communication technologies and transformation of survey research in social sciences Dr. Marko Grobelnik
- Quality of service and quality of experience measurement and control system in

## MENTORING

### Ph. D. Theses

- Blaž Fortuna, Semi-automatic ontology construction (mentor Dunja Mladenić).
- Inna Novalija, Ontology extension using text mining for news analysis (mentor Dunja Mladenić)

### Bologna M. Sc. Thesis

Alexandra Moraru, Enrichment of sensor descriptions and measurements using 1. semantic technologies (mentor Dunja Mladenić).

# VISITORS FROM ABROAD

- Vin de Silva, Department of Mathematics, Pomona College, Claremont, California, USA, 1. 8-12 January 2011
- 2 Abraham Hsuan, Irwin & Hsuan Ltd., New York, USA, 10-14 January 2011
- 3 Dr. Mark Pleško, Cosylab d.o.o., Ljubljana, 24 January 2011
- 4. Andraž Tori, Zemanta d.o.o., Ljubljana, 7 February 2011
- Bojan Blažica, Xlab d.o.o., Ljubljana, 16 February 2011 5
- 6. Dr. John Davies, British Telecom, United Kingdom, 20-22 February 2011
- Ian Thurllow, British Telecom, United Kingdom, 20-22 February 2011
- 8 Ass. Prof. Michelangelo Ceci, University of Bari, Italy, 4 March 2011
- 9. Sandi Klavžar, University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, 3 March 2011
- 10. Pavle Saksida, University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, 3 March 2011
- 11. Andrej Kastrin, Faculty of Information Studies, Novo Mesto, 3 March 2011
- 12. Janez Povh, Faculty of Information Studies, Novo Mesto, 3 March 2011
- 13. Ass. Prof. Yannis Charalabidis, University of AEGEAN, Greece, 3-5 March 2011
- 14. Blaž Golob, Centre for eGovernance Development, Ljubljana, 3-5 March 2011
- 15. MSc. Rayid Ghani, Accenture, Chicago, USA, 22-25 March 2011

## STAFF

#### Researchers

- Dr. Damjan Bojadžiev 1.
- 2. Asst. Prof. Branko Kavšek\*
- Dr. Gregor Leban<sup>3</sup>
- Prof. Dunja Mladenić, Head 4.
- Asst. Prof. Iztok Savnik\* 5.
- 6. John Stewart Shawe-Taylor, B. Sc.
- Dr. Primož Škraba

### Postdoctorial associates

- 8. Dr. Jurii Leskovec
- 9. Dr. Andrej Muhič\*
- Postgraduates
- 10. Luka Bradeško, B. Sc. 11 Janez Brank M Sc.
- 12. Dr. Blaž Fortuna
- 13. Ravid Ghani, M. Sc.
- 14. Mitja Jermol, M. Sc.
- 15. Simon Krek\*, B. Sc.
- 16. Blaž Novak, B. Sc.
- 17. Dr. Inna Novalija

multimedia communications environments Asst Prof Marko Grobelnik

- Co-authorship networks of slovenian scholars: Theoretical analysis and visualization 3 user interface development
- Prof. Dunja Mladenić 4. Slovene Research Atlas Prof. Dunja Mladenić

### RESEARCH PROGRAM

- Knowledge Technologies 1. Prof. Nada Lavrač
- 16. Pierre Bonnard, IdeXlab, France, 10 May 2011
- 17. Abraham Hsuan, Irwin & Hsuan Llp., New York, USA, 2-8 June 2011
- Ass. Prof. Tina Eliassi-Rad, Rutgers University, New Jersey, USA, 3-4 June 2011
- 19. Ass. Prof. Brandon Fitelson, Rutgers University, New Jersey, USA, 3-4 June 2011
- 20. Gil Ha, Grenhill, New York, USA, 5-7 June 2011
- 21. Prof. Mirjana Ivanović, University of Novi Sad, Faculty of Science, Serbia, 6-10 June 2011 22. Teac. Ass. Dr. Miloš Radovanović, University of Novi Sad, Faculty of Science, Serbia,
- 6-10 June 2011 23. Res. Ass. MSc. Doni Pracner, University of Novi Sad, Faculty of Science, Serbia, 6-10
- June 2011 24. Prof. Dr. Grigoris Antoniou, University of Crete, Greece, 10 June to 1 July 2011
- 25. Pierre Bonnard, IdeXlab, France, 1 September 2011
- 26. Prof. Colin de la Higuera, Nantes University, France, 1-2 September 2011
- Prof. Steve Gunn, University of Southampton, United Kingdom, 2 September 2011 27
- Res. Admi. Rebecca Martin, University College London, United Kingdom, 2 September 2011
   Schulte Olaf, ETH Zürich, Switzerland, 2 September 2011
- 30.
- Prof. Neil Lawrence, University of Sheffield, United Kingdom, 2 September 2011 Rok Sosič, SkyGrid, California, USA, 6 September 2011
- 31.
- Ying Sosič, Altera Corporation, California, USA, 6 September 2011 32
- 33. Ass. Prof. Oscar Corcho, Universidad Politécnica de Madrid, Spain, 22 September 2011 Prof. Dr. Mirjana Ivanović, University of Novi Sad, Faculty of Science, Serbia, 9-12 34. October 2011
- 35
- Dr. Zoran Budimac, University of Novi Sad, Faculty of Science, Serbia, 9–12 October 2011 Abraham Hsuan, Irwin & Hsuan Llp., New York, USA, 9–13 October 2011 36
- 37. Dr. Miloš Radovanović, University of Novi Sad, Faculty of Science, Serbia, 9-15 October 2011
  - 38. Mag. Doni Pracner, University of Novi Sad, Faculty of Science, Serbia, 9-15 October 2011
- Dr. John Davies, British Telecom, United Kingdom, 11 October 2011 39.
- 40. Michael Witbrock, Cycorp, USA, 17 October 2011
- Dr. Irena Nančovska Šerbec, University of Ljubljana , Faculty of Education, Ljubljana, 17 41. October 2011
- 42. Michael Witbrock, Cycorp, USA, 28 November to 2 December 2011
- Abraham Hsuan, Irwin & Hsuan Llp., New York, USA, 28 November to 2 December 2011
- Nuria Valles Peris, FIAS Foundation, Barcelona, Spain, 12 December 2011 44.
- 45. Nadine Dittert, Technologie-Zentrum Informatik und Informationstechnik, Universität Bremen, Germany, 12 December 2011

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- 18. Jan Rupnik, B. Sc.
- 19. Tadej Štajner, B. Sc.

#### 20. Mitja Trampuš, B. Sc. **Technical officers**

- 21. Dr. Sabrina Guettes, left 01.03.11
- 22. Matjaž Rihtar, B. Sc.
- 23. Janez Starc, B. Sc.
- 24. Jasna Škrbec, B. Sc.
- 25. Maja Škrjanc, B. Sc.
- 26. Aleš Špetič. B. Sc.
- Technical and administrative staff
- 27. Marko Grobelnik
- 28 Klemen Kenda
- 29. Mojca Kregar Zavrl, B. Sc.
- Boštjan Pajntar
- 31. Mateja Zver

Note:

\* part-time JSI member

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### TEXTBOOKS AND LECTURE NOTES

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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 2011, 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", "INSARTY" and "UNITE", the eContentplus "ICOPER" and "OpenScout" projects, 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 work 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.

#### 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 connotation 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 the low-cost delivery of professional and user-created content. In 2011 the laboratory's contribution to the project was focused on security-services provisioning in such systems, enhancements of the JSI/RTV Living lab content ingest and additional video-on-demand (VoD) services and their management. Contributions have resulted in software components of the project Next-Share platform, namely ProviderToolbox, implementing VoD and live stream ingest, RichMetadata, implementation of the project-defined content metadata specification, Monitoring, a platform for supervising content ingest and distribution, and Enhanced Closed Swarm protocol, enabling flexible and context aware access control to BitTorrent distribution channels.

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 research of the Future Internet.

Under the Infrastructure program in research organizations we have upgraded in 2011 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 multidisciplinary 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.

#### **Technology enhanced learning**

An important part of our research activities deals with technology-enhanced learning and education. In the frame of the "Interoperable Content for Performance in a Competency-driven Society (**ICOPER**)" project from the European eContentplus programme, we successfully concluded research on learning outcomes and competences in technology-enhanced higher education. The project evaluated the existing standards, such as IEEE RCD, IMS LD or IMS QTI, for learning outcome-based education and described good practices in the specification and formal description of the learning outcomes, searching for the most useful courses according to the expected learning outcomes, the evaluation of the obtained skills and competencies, and the collection of learner achievements over longer periods of time. In 2011 we analysed the whole learning-outcome-based education domain at the concept levels. The comparison was made among the various concept models developed for the competency domain, by



Prof. Borka Jerman Blažič

different groups, and from different perspectives. As a result of this comparison, a meta-model was produced as a suggested conceptual framework for the domain. Recommendations from the analysis of the gaps between the current situation and the desired futures described in both the context and the future scenarios were also given. This work presents the list of gaps and the respective recommendations in the final ICOPER road-mapping document. In cooperation with other project partners we finalized the ICOPER reference model that defines the basic concepts and their relations, technical services and processes in learning-outcome-based learning. The standardisation of



Figure 1: Researchers Night 2011 in Ljubljana and Novo mesto

our formal PALO (Personal Achieved Learning Outcomes) specification also started in 2011 within CEN WS/LT (CEN Workshop on "Learning Technologies"). Part of the eContentplus programme is also the "Skill-based scouting of open user-generated and community-improved content for management education and training (**OpenScout**)" project that enables users to easily find, access, use and exchange open content for management education and training. The open content can be found, retrieved from or published at the learn.openscout.net portal.

At the end of 2011 we started with our new project **SELPRAF** "Selfemployment with e-leaning based Practise Firms" (Leonardo da Vinci). The general aim of SELPRAF 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 the 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.

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.

#### Security, dependability and privacy in information systems

The provision of security and privacy services is crucial for the modern information society. In 2011 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., as well as on secure applications, e.g., graphical authentication systems. The problems were approached in a multidisciplinary way. The first area of research was trust and reputation management in P2P networks and social software systems. We have defined a novel reputation systems taxonomy that takes into account the human-centric way of establishing trust brought by the impression management and the business performance from social interactions. The results were presented as an invited paper at the Future Internet week and Assembly, the ServiceWave conference, later published in Computer Lecture Notes. The second area of research was related to authorization and access control in P2P networks. Within the previously mentioned "P2P-Next" project we updated a content-delivery system based on the BitTorrent protocol named Closed Swarms and its extension, the Enhanced Closed Swarms. The protocol allows us to differentiate between authorized and non-authorized nodes (peers) within an overlay network. In 2011 we extended the Enhanced Closed Swarms protocol for distributed access control in P2P networks with options that enable the content provider (TV broadcaster) to create and maintain a hierarchical structure of seeds in order to achieve fine-grained load balancing and optimization of the delivery process. The extension provides more flexible access control and enables new scenarios and business models of video-content distribution in P2P networks. The enhanced protocol was integrated into the P2P-Next delivery platform and the results were presented at the scientific conference Securware 2011, where our paper received the best paper award.

Research and practice in past years have shown that security problems that arise because of the low level acceptance of security solutions by the end user can be solved only by considering the usability perspective of the user. In an attempt to create more memorable authentication mechanisms, several approaches based on graphical and image passwords have been devised recently, where the authentication is based on image clicking as opposed to typing character-based passwords. In 2011 we published a paper in an SCI journal on a novel graphical recognitionbased authentication system that is both secure and usable. The system is especially suitable for the authentication of users with mobile devices with touch-screen interfaces.

#### **Science promotion**

In September 2011 we successfully organized **Researcher's Night 2011**. INSARTY (Introducing Science and Art to Slovenian Youth and Citizens) was a 7-month project proposed by the Jožef Stefan Institute in collaboration with Faculty of Information Studies, Novo mesto, to reach the specific objective of bringing researchers closer to the public at large through the organization and holding of the 2011 Researcher's Night in the area of Ljubljana (Prešeren Square, Jožef Stefan Institute, Prešernova street) and Novo mesto (Janez Trdina Cultural Centre) on Friday, 23 September 2011. Additionally, the 20th Anniversary of first internet line in Slovenia, that was part of European EUREKA-8 COSINE project (1988 – 1992) and was set up by Laboratory for Open Systems and Networks and the NIKHEF institute from Amsterdam in 1991, celebration and the regional R&D and youth researcher Nahtigalova's awards ceremonies were integrated into the programme of the project to stress the significance of the event and to attract as many visitors as possible. We estimated total number of visitors at all venues to be between 3000 and 4000. This high level of interest was reflected in over 23,000 visits the webpage and 754 "Likes" on Facebook.

#### Some outstanding publications in the past three years

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### Organization of conferences, congress and meetings

- 1. The 2011 Researcher's Night, 23 September.
- 2. Anniversary of the first 20 years of the Internet's connection in Slovenia, 23 September.

#### Awards and appointments

1. Vladimir Jovanovikj, Dušan Gabrijelčič, Tomaž Klobučar: Best paper award at SECUREWARE 2011, The Fifth International Conference on Emerging Security Information, Systems and Technologies, Nice – Saint Laurent du Var, France, 21–27 August 2011.

# INTERNATIONAL PROJECTS

- 1. Introducing Science and Art to Slovenia Youth in Citizens 7. FP , 287453
  - EC Prof. Borka Jerman Blažič
- Upgrading ICT Excellence by Strengthening Cooperation between Research Teams in an Enlarged Europe
  - UNITE
  - 7. FP , 248583

EC; Ricardo Goncalves, UNINOVA - Instituto de Desenvolvimento de Novas Technologias, Monte Caparica, Portugal

- Prof. Borka Jerman Blažič
- 3. Next Generation Peer-to-Peer Content Delivery Platform P2P-Next
  - 7. FP, 216217

EC; Jari Ahola, VTT - Valtion Teknillinen Tutkimuskeskus, Espoo, Finland Dr. Dušan Gabrijelčič

- 4. Towards the Integration of Trans-sectorial IT Design and Evaluation COST IC0904
- EC

Matija Pipan, M. Sc.

- Self-employment with e-Leaning based Practise Firms SELPRAF
  - Leonardo da Vinci Programme

Center Republike Slovenije za mobilnost in evropske programe izobraževanja in usposabljanja - CMEPIUS, Ljubljana, Slovenia; Srednja ekonomska šola Celje, Celje, Slovenia Dr. Tania Arh

 Skill based Scouting of Open User-generated and Community-improved Content for Management Education and Training OpenScout eContentplus

ECP-2008-EDU-428016 EC; Jyväskylän Yliopisto, University of Jyväskylän, Jyväskylä, Finland Asst. Prof. Tomaž Klobučar

- 7. Interoperable Content for Performance in a Competency-driven Society ICOPER
- eContentplus ECP-2007-EDU-417007

EC; Dr. Bernd Simon, Wirtschaftsuniversität Wien, Institut für Wirtschaftsinformatik und Neue Medien, Vienna, Austria Asst. Prof. Tomaž Klobučar

## R & D GRANTS AND CONTRACTS

- 1. Security , dependability and privacy in pervasive systems Prof. Borka Džonova Jerman Blažič
- Security and trust in the new generation of P2P networks Prof. Borka Džonova Jerman Blažič
- Future Internet collaboration platform Prof. Borka Džonova Jerman Blažič

## RESEARCH PROGRAM

 Future Internet Technologies: concepts, architectures, services and socio-economic issues Prof. Borka Džonova Jerman Blažič

# **MENTORING**

### Ph. D. Theses

1. Rok Bojanc, Models for providing security in business information systems (mentor Borka Jerman Blažič).

# VISITORS FROM ABROAD

- Msc. Martin Mihajlov, Faculty of Economics, Cyril and Methodius University in Skopje, Skopje, Macedonia, 2-4 November 2011.
- Martin Mihajlov, Usable authentication with recognition-based graphical passwords (mentor Borka Jerman Blažič; co-mentor Tomaž Klobučar).
- Prof. Vladislav V. Fomin, Faculty for Informatics, University Vytautas Magnus, Kaunas, 2. Lithuania, 8 December 2011.
- Dr. Mark Springett, Middlesex University, Great Britain, 13 December 2011 3.

### STAFF

#### Researchers

### 1. Prof. Borka Džonova Jerman Blažič, Head

- Asst. Prof. Tomaž Klobučar Postdoctorial associates

#### Dr. Tanja Arh 3. Dr. Dušan Gabrijelčič

- Postgraduates
- Tania Ažderska, B. Sc.

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- 1. Tanja Ažderska, Borka Jerman-Blažič, "A novel systemic taxonomy of trust in the online environment", In: Towards a service-based internet: 4th European conference, ServiceWave 2011, Poznan, Poland: proceedings, Lect. notes comput. sci., vol. 6994, pp. 122-133, 2011.
- 2. Borka Jerman-Blažič, "Four scenarios for future evolution of the
- internet", *IEEE technol. soc. mag.*, vol. 30, no. 4, pp. 39-46, 2011. 3. Martin Mihajlov, Borka Jerman-Blažič, "On designing usable and secure recognition-based graphical authentication mechanisms", Interact. comput., vol. 23, no. 6, pp. 582-593, 2011.

### **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

- 1. Tanja Arh, Vlado Dimovski, Borka Jerman-Blažič, "ICT and web 2.0 technologies as a determinant of business performace", In: Cases on ICT utilization, practice and solutions: tools for managing day-to-day issues, Mubarak S. Al-Mutairi, ed., Lawan Ahmed Mohammed, ed., Hershey, New York, Information Science Reference, cop. 2011, pp. 59-77.
- 2. Tanja Arh, Dejan Dinevski, "Web 2.0 and open educational resources as a foundation of organisational learning", In: People and sustainable organization, Tomaž Kern, ed., Vladislav Rajkovič, ed., Frankfurt am Main [etc.], Peter Lang, 2011, pp. 44-62.
- 3. Tomaž Klobučar, "E-izobraževanje in učni izidi", Mednarodno inovativno poslovanje, vol. 3, no. 2, 2011.

### PUBLISHED CONFERENCE PAPERS

### **Regular** papers

- 1. Tanja Arh, Borka Jerman-Blažič, "An assessment of the usability of the Virtual Conference Centre Global Plaza and the associated social network", In: ED-MEDIA 2010: world conference on educational multimedia, hypermedia & telecommunications June 27, 2011, Lisbon, Portugal, (EMEDIA, vol. 2011, no. 1, 2011), Chesapeake, AACE, 2011, pp. 1486-1494.
- 2. Tanja Arh, Rok Kokalj, "Priporočila in izhodišča za pripravo e-učnega gradiva", In: Organizacija prihodnosti: zbornik 30. međnarodne konference o razvoju organizacijskih znanosti, Slovenija, Portorož, 23.-

Andrej Jerman Blažič, M. Sc. 6. Vladimir Jovanovikj, B. Sc. 8 Maks Mržek, B. Sc. Matija Pipan, M. Sc. **Technical officers** 10. Primož Cigoj, B. Sc. Technical and administrative staff 11. Tatiana Martun, B. Sc.

> 25. marec 2011: proceedings of the 30th International Conference on Organizational Science Development, 30. mednarodna konferenca o razvoju organizacijskih znanosti, Slovenija, Portož, 23.-25. marec 2011, Marko Ferjan, ed., Mirjana Kljajić Borštnar, ed., Andreja Pucihar, ed., Kranj, Moderna organizacija, 2011, pp. 9-20.

- 3. Tanja Arh, Marija Mojca Peternel, Matija Pipan, Borka Jerman-Blažič, "Increasing the penetration of the unemployed into the labour market with e-learning based practice firms in Slovenia and Croatia", In: Recent researches in circuits, systems, communications and computers: proceedings of the 2nd European Conference of Systems, (ECS '11), 2nd European Conference of Circuits Technology and Devices, (ECCTD '11), 2nd European Conference of Communications, (ECCOM '11), 2nd European Conference of Computer Science, (ECCS '11), December 10-12, 2011, Puerto De La Cruz, Tenerife, Spain, Nico Mastorakis, ed., [S. l.], WSEAS, World Scientific and Engineering Academy and Society, cop. 2011, pp. 279-284.
- 4. Tanja Ažderska, Borka Jerman-Blažič, "Online trust and reputation: towards socially aware taxonomy of trust", In: 1st unite doctoral symposium, 27th - 29th june, University Politehnica of Bucharest, (Unite Doctoral Symposium), Ricardo Jardim-Gonçalves, ed., Guy Doumeingts, ed., Aurelian Mihai Stanescu, ed., Bucharest, Editura Printech, 2011, pp. 79-85.
- 5. Igor Balaban, Goran Bubas, Matija Pipan, "Key elements of an elearning course evaluation survey: an empirical validation", In: Proceedings, 14th International Conference on Interactive Collaborative Learning (ICL2011) [and] 11th International Conference Virtual University (vu'11), 21-23 September 2011, Piešt'any, Slovakia, Bratislava, Faculty of Electrical Engineering and Information Technology, 2011, pp. 336-343.
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- 7. Borka Jerman-Blažič, "Prihod prve internetne linije v Slovenijo. 2. del", In: Zbornik 14. mednarodne multikonference Informacijska družba - IS 2011, 10.-14. oktober 2011: zvezek A: volume A, (Informacijska družba),

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- 9. Vladimir Jovanovikj, Dušan Gabrijelčič, Tomaž Klobučar, "Access control in BitTorrent P2P networks uisng the enhanced closed swarms protocol", In: *Netware 2011: August 21-27, 2011, French Riviera, Nice*-*Saint Laurent du Var, France*, [S. l.], IARIA, cop. 2011, pp. 97-102.
- 10. Vladimir Jovanovikj, Dušan Gabrijelčič, Tomaž Klobučar, "Access control in BitTottent P2P networks using the enhanced closed swarms protocol", In: *Zbornik prispevkov*, 3. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 3rd Jožef Stefan International Postgraduate School Students Conference, 25. maj 2011, Ljubljana, Slovenija, Dejan Petelin, ed., Aleš Tavčar, ed., Brigita Rožič, ed., Bogdan Pogorelc, ed., Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2011, pp. 68-73.
- Vladimir Jovanovikj, Dušan Gabrijelčič, Tomaž Klobučar, "Context modelling in context-aware security systems", In: *Zbornik dvajsete mednarodne Elektrotehniške in računalniške konference ERK 2011, 19.-*21. september 2011, Portorož, Slovenija, (Zbornik ... Elektrotehniške in računalniške konference ERK ...), Baldomir Zajc, ed., Andrej Trost, ed., Ljubljana, IEEE Region 8, Slovenska sekcija IEEE, 2011, zv. B, pp. 51-54.
- 12. Martin Mihajlov, Borka Jerman-Blažič, Sašo Josimovski, "Quantifying usability and security in authentication", In: *Proceedings: COMPSAC* 2011, 35th Annual IEEE International Computer Software and Applications Conference, 18-21 July 2011, Munich, Germany. Vol. 1, Main conference, (Proceedings - International Computer Software & Applications Conference), COMPSAC 2011, 35th Annual IEEE

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- 14. Jad Najjar, Tomaž Klobučar, Ang Vu Nguyen-Ngoc, Michael Totschnig, Franz Müller, Bernd Simon, Mikael Karlsson, Henning Eriksson, "Towards outcome based learning: an engineering education case", In: *IEEE EDUCON 2011: [proceedings]*, IEEE Engineerng Education Conference, 4-6 April 2011, Amman, Jordan, Michael E. Auer, ed., [S. l., s. n.], cop. 2011, pp. 1039-1048.
- Matija Pipan, "Designing usability evaluation methodology in the case of openscout portal", In: *Proceedings*, Danijela Milošević, ed., Belgrade, Belgrade Metropolitan University, 2011, pp. 38-42.
- 16. Matija Pipan, "Na veščinah in kompetencah temelječe iskanje prosto dostopnih e-vsebin s področja managementa", In: Organizacija prihodnosti: zbornik 30. mednarodne konference o razvoju organizacijskih znanosti, Slovenija, Portorož, 23.-25. marec 2011: proceedings of the 30th International Conference on Organizational Science Development, 30. mednarodna konferenca o razvoju organizacijskih znanosti, Slovenija, Portož, 23.-25. marec 2011, Marko Ferjan, ed., Mirjana Kljajić Borštnar, ed., Andreja Pucihar, ed., Kranj, Moderna organizacija, 2011, pp. 1038-1044.

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1. Andrej Jerman Blažič, *Educational web applications in vocational education and training in Slovenia:* master's thesis, Ljubljana, [A. Jerman Blažič], 2010.

# DEPARTMENT OF COMMUNICATION **SYSTEMS** E-6

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 the 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 medical surgery procedures and specialised equipment and procedures for advanced bio-signal processing.

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 particularly reflected in the joint applied projects.

In 2011 the research activities within the Communication Technology Laboratory were concentrated on Head: different challenges associated with the access segment technologies enabling the end-users to access new mul- Asst. Prof. Mihael Mohorčič timedia services and applications. As part of the multi-year telecommunication-systems research programme the emphasis was on the research in the areas of: radio propagation, multiple input multiple output (MIMO) antenna systems, 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 mobile-communications 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).

We continued the research of the utilization of wireless-communication technologies in mesh networks. For this purpose we developed and implemented a software tool called TopoSWiM for topology design and accessibility provision in large-scale wireless mesh networks, combining the mathematical approach based on the graph theory with a physical model of an operating environment and of signal propagation. The tool provides large flexibility in terms of simulation parameters and scenarios, a user-friendly visualization of the generated topology and a comparison of the topologies for different network settings in near-real time.

The activities in the area of fixed mobile convergence were focused on the mobility management in convergent networks, in particular, on the seamless vertical handover between the networks based on different access technologies. 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 investigated advanced concepts and technologies for a capacity increase of wireless meshed networks using the network coding techniques. In order to support performance evaluation of the arbitrary network coding algorithms on predetermined or randomly generated topologies of wireless meshed networks, we designed and built a simulation model.

In the framework of the COST IC0802 project and in cooperation with the French Aerospace Lab ON-ERA we developed new methods for processing satellite beacon data received from EUTELSAT HotBird 6. Related to this activity we also obtained the ESA PECS project "Ka/Q-band Propagation Measurements and Modelling for the Design of Prediction and Impairment Mitigation Techniques" (SatProSi), which includes multidisciplinary aspects of wireless also the development of our own Beacon Receiver for EUTELSAT HotBird 6 signal.

In 2011 we joined COST Action IC1101 "Optical Wireless Communications - An Emerging Technology". Within this COST Action and in cooperation with TU Graz we are developing new channel models for terrestrial free-space optical links.





networks entitled "Application and sensor networks: concepts, integration, and case studies", with Roman Trobec as a co-editor and a contribution on body sensors prepared by Ivana Tomašić and Roman Trobec.

- For the integration in open-source geographic information systems GRASS, we developed and implemented a software module for the 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 a modular and fully flexible platform VESNA for the research and implementation of wireless sensor networks.

In the area of cognitive communications we continued the research in the radio and access segments and contributed to the projects WUN-CogCom and COST IC0902. In the access segment we were focusing on the development of the procedures for semi-automated and automated protocol stack compositions, whereas in the radio segment we developed a low-cost, energy-detection-based, radio-frequency-spectrum sniffer. It can be used for a stand-alone spectrum sensing in cognitive radio terminal or in collaborative sensing for building a space-time frequency spectrum utilisation database.

In cooperation with the Department of Low and Medium Energy Physics (F2) we improved the method for a short-range quantum key distribution. The method extends classical cryptographic schemes with the possibility to exchange a shared secret key between the two parties using the quantum effects in a way that guarantees unconditional security. Common research activities also focused on the high-data-rate acquisition in the detector systems and on the efficient signal processing algorithms.

In the Parallel and Distributed Systems Laboratory, we successfully

Figure 2: Open-source radio planning tool GRASS-RaPlaT

Engineering and the Laboratory for Algorithms and Data Structures from the Faculty of Computer and Information Science. We were heavily involved in the research within the program Parallel and Distributed Computing and also in other research projects. Our cooperating researchers also come from the industry (Turboinstitut d.d. and Xlab d.o.o.) and from the medical sphere (the University Clinical Center Ljubljana).

We investigated computer algorithms for efficient implementation on parallel and distributed computers, testing them on a 37-processor 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 data storing. 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 numeric 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 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

continued the interdisciplinary research work in the framework of an enhanced program group, as we were joined by the colleagues from the University of Ljubljana, the Machine Vision Laboratory from the Faculty of Electrical

> optimizations and began to investigate how to efficiently integrate measurement results, simulation results and optimization methods, which will enable us to predict biological parameters not obtainable 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 the 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, proposing improved algorithms and stronger state-recognition principles. We also investigated the communication protocol verification, proposing transformations for simplifying the behaviour specification of individual partners without influencing the syntactical errors of the protocol.



Figure 3: VESNA platform for the research and implementation of wireless sensor networks

In 2011 the Networked Embedded Systems Laboratory mainly focused on research and development in the area 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 conducted, in part, within the basic research project "Advanced procedures for interactive composition of sensor networks" and, in part, in the EU 7FP Network of Excellence PlanetData.

The design and development of a modular and fully flexible platform VESNA for wireless sensor networks represents one of the main results of the laboratory in 2011. Different combinations of developed modules and supported technologies make the platform well suited for the implementation of the experimental sensor networks required in basic or applied research, as well as for the deployment of tailor-made applications.

In collaboration with the Municipality of Logatec we started to build an experimental sensor-network testbed LOG-a-TEC to be used in different basic and applied projects. The testbed is based on the use of the VESNA platform, which will be equipped according to the requirements of a given project with different sets of sensors and communication modules for the transmission of the measurements to the central database. As part of the LOG-a-TEC testbed we are building a sensor network for the 7FP CREW project and the FIRE initiative, which will enable an experimentally-driven research in the areas of spectrum sensing in licensed and unlicensed frequency bands, cognitive radio and cognitive networking. The LOG-a-TEC testbed will be the only one of the 5 CREW testbeds to support the investigation of horizontal and vertical radio-spectrum-sharing methods in a real-life outdoor environment.

Our research work in the frame of the 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 the sensor networks to the management services and applications. To this end, we are developing different sensor modules, investigating procedures for preprocessing of data and metadata, and developing the required interfaces to the platform. We also developed a discovery and identification protocol (DIP) for discovering sensor resources and data delivery.

In the area of wireless sensor networks we successfully finished the EU 7FP project AgroSense and started a new 7FP project BalkanGEONet. We designed a remotely controlled airplane model with an autopilot and developed software and hardware equipment for the remote collection, transmission and processing of the sensor data and images.

The Networked Embedded Systems Laboratory and its research activities are also part of the interdepartmental laboratory SensoLab, established together with the Laboratory of Artificial Intelligence (E3).

### Some outstanding publications in the past year

- 1. Mohammed Abbas, Mehmood Asad, Fotini-Niovi Pavlidou, And Mohorčič Mihael. The role of high-altitude platforms (HAPs) in the global wireless connectivity. Proc. I.E.E.E., 2011, vol. 99, no. 11, 1939-1953.
- Celcer Tine, Kandus Gorazd, Javornik Tomaž. Adaptive utility-based scheduling algorithm for multiuser MIMO uplink. EURASIP J. wirel. commun. netw. (online), 2011, vol. 2011, no. 22, pp. 1-12. http://jwcn.eurasipjournals.com/content/2011/1/22, doi: 10.1186/1687-1499-2011-22.
- Trobec Roman, Tomašić Ivan. Synthesis of the 12-lead electrocardiogram from differential leads. IEEE trans. inf. technol. biomed. 15, 2011. 615-621.

- For the needs of different projects we are building an experimental sensor-network testbed LOG-a-TEC supporting the ondemand dynamic composition of sensor and communication resources.
- In the frame of the EU 7FP CREW project and the FIRE initiative the LOG-a-TEC testbed will be used as a real-life outdoor experimental environment for cognitive radio and cognitive networking research.
- We have compared calculation complexities of different meshless methods for solving a diffusion equation and concluded that strongly formulated approaches are computationally more efficient than weak formulations.



Figure 4: Optimal gateway locations, estimated by TopoSWiM, a software tool for topology design of large-scale wireless mesh networks



Figure 5: Average temperatures of all the patients during a cooling treatment in Group A with the gel-pack (left) and Group B with the cTreatment® (right). Abbreviations: ICN- intercondylar notch, SC - subcutaneous, SK - skin (12 - anterior, 3 - medial, 6 - posterior, 9 - lateral), BA - bandage.

- We have developed a prototype wireless electrode of biopotentials from the body surface for the concurrent measurements of the ECG and the respiration rate.
- We synthesised, with a high reliability, a standard 12-lead ECG from three bipolar wireless electrodes.
- We developed a simulation model for performance evaluation of the network coding techniques.



Figure 6: Target (blue) and synthesized (red) 12-lead ECG. The measurement is taken five days after a CABG surgery. Minimal CC is 0.971 for lead III and maximal RMS error is 41.9 µV for lead I.

# INTERNATIONAL PROJECTS

- 1. Cognitive Radio Experimentation World
  - CREW
  - 7. FP, 258301

EC; Ingrid Moerman, Interdisciplinary Institute for Broadband Technology (IBBT vzw), Ledeberg, Belgium

- Asst. Prof. Mihael Mohorčič Balkan GEO Network - Towards Inclusion of Balcan Countries into Global Earth
- Balkan GEO Network Towards Inclusion of Balcan Countries into Global Eart Observation Initiatives BalkanGEONet
  - 7. FP. 265176

EC; Prof. Vladimir Crnojević, University of Novi Sad, Novi Sad, Serbia

- Asst. Prof. Mihael Mohorčič
- 3. Planet Data
- 7. FP, 257641

EC; Alice Carpentier, Dieter Fensel, Universitaet Innsbruck, Innsbruck, Austria

Asst. Prof. Mihael Mohorčič, Marko Grobelnik, Prof. Dunja Mladenić, Mitja Jermol, M. Sc.

- 4. Enabling the Knowledge Powered Enterprise
  - ACTIVE
  - 7. FP, 215040

EC; Philip Hewitt, British Telecommunications plc, London, Great Britain Asst. Prof. Mihael Mohorčič, Mitja Jermol, M. Sc., Marko Grobelnik, Prof. Dunja Mladenić

- 5. Trans-national Cooperation among ICT NCPs
  - IDEALIST2011
  - 7. FP, 231367

EC; Deutsches Zentrum für Luft- und Raumfahrt E. V. (DLR), Köln, Germany Asst. Prof. Mihael Mohorčič

- 6. Wireless Sensor Networks and Remote Sensing Foundation of a Modern Agricultural Infrastructure in the Region
  - AgroSense 7. FP, 204472
  - 7. FP, 2044/2
  - EC; University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Serbia
- Prof. Kandus Gorazd, Asst. Prof. Mihael Mohorčič 7. Cooperative Radio Communications for Green Smart Environments
- . Cooperative Radio Communications for Green Smart Environment

 Kosec Gregor, Založnik Miha, Šarler Božidar, Combeau Hervé. A meshless approach towards solution of macrosegregation phenomena. Computers, materials & continua, 22, 2011, 169-195

### Patent granted

 Method for synthesis of magnetic liposomes in electric field Kristina Eleršič, Miran Mozetič, Alenka Vesel, Janez Pavlič, Aleš Iglič, Andrej Žnidaršič, Aljoša Košak SI23095 (A), Urad RS za intelektualno lastnino, 31.1.2011.

### Organization of conferences, congress and meetings

1. Co-organization of the meeting: BalkanGeoNet – Earth Observations for the Social Benefit of the Balkans Post-GEO Workshop, Istanbul, Turkey, 17.11.-22.11.2011



Figure 7: Results of numerical simulation of a binary material solidification (Sn-10%Pb). Concentration and velocity fields are presented at the moment when the instabilities appear (left), and in the steady state (right). In the steady state the mesosegretaes, which are still not understood, are visible (the areas filled with a high concentration).

COST IC1004 EC; COST Office, Brussels, Belgium Asst. Prof. Tomaž Javornik Optical Wireless Communications - An Emerging Technology 8. COST IC1101 EC; COST Office, Brussels, Belgium Prof. Gorazd Kandus, Asst. Prof. Tomaž Javornik Wireless Networking for Moving Objects WiNeMO COST IC0906 EC; COST Office, Brussels, Belgium Miha Smolnikar, Asst. Prof. Aleš Švigel 10. Cognitive Radio and Networking for Cooperative Coexistence of Heterogeneous Wireless Networks COST IC0902 EC; COST Office, Brussels, Belgium Asst. Prof. Mihael Mohorčič, Miha Smolnikar 11. Open European Network for High Performance Computing on Complex Environments CÔST ICO805 EC; COST Office, Brussels, Belgium Prof Roman Trobec 12. Propagation Tools and Data for Integrated Telecommunication, Navigation and Earth Observation Systems COST IC0802 EC; COST Office, Brussels, Belgium Prof. Gorazd Kandus, Dr. Andrej Vilhar 13. Processing of Satellite Signals in Ka/Q-frequency Band SatProSi ESA PECS 4000104510/11/NL/KML Bernard Zufferey, ESA-The European Space Agency, Paris, France; European Space Research and Technology Centre, Noordwijk, The Netherlands Prof. Gorazd Kandus Study Relating to the Measurement of the Effects of Cryotherapy on a Human Body 14 Research Agreement

Konrad Lang, Levi Dewaegenaere, Waegener Research & Development N.V., Beerse, Belgium Prof. Roman Trobec

## **R&D GRANTS AND CONTRACT**

- 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 compositional visual architecture Prof. Roman Trobec
- Multiantena Systems for mobile WiMAX Prof. Gorazd Kandus

### MENTORING

### Ph. D. Thesis

1. Andrej Hrovat, Radio wave propagation in special environments (mentor Gorazd Kandus; co-mentor Tomaž Javornik).

#### Bologna M. Sc. Thesis

 Maria Porcius, Topology design and accessibility provision in large scale wireless mesh networks (mentor Mihael Mohorčič).

## RESEARCH PROGRAMS

- 1. Telecommunication Systems
- Prof. Gorazd Kandus 2. Parallel and Distributed Systems Prof. Roman Trobec

### NEW CONTRACTS

- Analytical and sensory support to the introduction of new services I Telekom Slovenije, d. d. Asst. Prof. Mihael Mohorčič
- Design and implementation of LTE radio coverage calculation modules for rural areas Telekom Slovenije, d. d.

Asst. Prof. Tomaž Javornik

### VISITORS FROM ABROAD

- 1. Dr. Farukh Nadeem, Tehnical University, Graz, Austria, June, 2011
- 2. Prof. Dr. Venčeslav Kafedjiski, Faculty of Electrotechnics, Skopje, Macedonia, 18. 7. 2011
- Patricia Oniga (internship), Technical University of Cluj-Napoca, Romania, 8. 7.–24. 9. 2011
   Melisa Junuzović (internship), Faculty of Electrotechnics, Tuzla, Bosnia and Hercegovina, 14. 7.–16. 9. 2011
- Dr. Nermin Suljanović, dr. Aljo Mijčić, Faculty of Electrotechnics, Tuzla, Bosnia and Hercegovina. 31, 8, 2011
- Dr. Patrick Millot in Dr. Laurent Castanet, Reasearch Institute ONERA, Toulouse, 6. 10. 2011
   Prof. Dr. Veljko Milutinović with colleagues, Faculty of Electrotechnics, Belgrade, Serbia, 4 11 2011
- 8. Prof. Dr. Musa Abidov, Medical University, Moscow, Russia, 23. 11. 2011

### STAFF

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- 14. Dr. Gregor Kosec
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#### Postgraduates

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- 22. Aleksandra Rashkovska, B. Sc.
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### PATENT

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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 particularly 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 world-wide, through academic and industrial links, thus enabling us to remain at forefront of this rapidly developing field.

In the field of computer structures we concentrate particularly on the design of FPGA-based reconfigurable systems for selected target applications. We also develop methods for on-line testing and a design of self-repairable systems.



In the area of hardware/software co-design we collaborate with the Faculty of Electrical Engineering and Computer Science, the University of Maribor. Within an application project we are developing a hardware accelerator for the compression of the LIDAR data. Last year the PCI-E interface of the arithmetic coder/decoder was developed. The PCI-E interface can achieve very high data-transfer throughput, especially if the DMA transfer mode is used. It Prof. Franc Novak was developed in the VHDL and Verilog languages and tested on a Xilinx XUPV5 prototype board. In addition, the device driver for the PCI-E interface was developed on the GNU Linux operating system. The implemented device driver supports the DMA mode transfers as well as the register and memory transfers. The device driver gives an

access to the input and output of the arithmetic coder as well as an access to the coder's internal data structure like the coding symbol probability distribution. The arithmetic coder and decoder are part of the overall architecture of the lossless compressor of LIDAR data; however, such implementation can also be used by other compression algorithms (i.e., lossy compression).

In another application, a compact 32-bit AES core including on-line error detection and an efficient built-in self-test suitable for small size FPGAs was developed. The implemented AES is specially designed for the FPGA-based embedded applications since it is tuned to specific FPGA logic resources. The on-line error detection is based on parity codes. This is the smallest AES core on FPGA with on-line error detection reported in the literature. In contrast to the other solutions that focus on individual AES processes (i.e., encryption, decryption, and key expansion) we perform an on-line test of complete AES. The low number of hardware resources and a considerably high data throughput make such an implementation suitable for small cryptographic cores in dependable embedded applications.

An important part of our research activities is related to the development of metaheuristic optimization methods and their applications. We have developed a differential ant-stigmergy algorithm (DASA) and its continuous variant (CDASA) and used them for the problem of parameter estimation of nonlinear dynamic systems represented by ordinary differential equations.



Figure 1: Examples of phase-contrast images of biological cells with a different cell density (from 126 cells/image - top right to 329 cells/ image - bottom left). The automatic procedure counts cells with over 90% accuracy.

More precisely, we addressed the problem of parameter estimation in a nonlinear dynamic model of an aquatic ecosystem (Lake Bled). We have also developed shared-memory and distributed-memory implementations of the

DASA algorithm suitable for solving continuous numerical optimization problems in multicore processor environment. The Intel-OpenMP 3.0 and MPICH2 libraries were used for the inter-thread and inter-process communications, respectively. In collaboration with the University of Salzburg, Austria, we conducted a study about the influence of simulation complexity on algorithm efficiency.

A part of our research activities in the field of optimization methods also

covers self-setting and self-adapting evolutionary algorithms. They were adapted for solving various combinatorial optimization problems. Their efficiency was tested with synthetic benchmark problems as well as real-world industrial problems.

We designed a compact, 32-bit, AES core suitable for embedded systems with limited hardware resources. This is the smallest AES core on FPGA with on-line error detection reported in the literature.

Within the industrial project for ETA Cerkno d.o.o., based on a successfully carried out pilot model, we have created an overall 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

We successfully applied metaheuristic algorithms for numerical optimization to the task of estimating the parameters in a model of the dynamics of the Rab5-to-Rab7 conversion in endocytosis. The results were published in the prestigious journal BMC Systems Biology.

for their own cooking appliances. So the production must be planned very carefully to fulfil all the demands (quantities and deadlines), to maintain the specified amount of different models in stock, to make best use of human resources, and to efficiently use all the production lines.

Within the project with Gorenje, d. d., Velenje, we developed a program tool for the simulation and optimization of temperatures inside refrigerators. Consequently, during the optimal functioning of a refrigerator the desired temperature is sustained with the lowest possible power consumption. With

a simulator that allows the simulation of the temperatures inside a refrigerator at different regulation modes, we replace the measurements that are time consuming due to the slow thermal processes. The integrated optimization algorithm automatically finds the optimal regulation of a refrigerator. On the basis of the measured temperature responses, the optimizer finds the optimal refrigerator control parameters. The developed tools substitute a several-day observation of a refrigerator with a several-second simulation. A large set of measurements thus becomes unnecessary and the development costs are significantly lowered.

In the area of machine vision we started a new project with the company Tesnila GK d.o.o., where the aim is to develop a quality-control machine-vision solution for various rubber parts produced by the company. The procedure



Figure 2: Development of hardware accelerator for the compression of LIDAR data

will include fast dimensional and surface inspection of each rubber part to replace 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 the electroporation treatment. The procedure was implemented in the software that will help researchers to quickly obtain the number of biological cells in a large number of image series. The tested accuracy is over 90%, which is comparable to manual counting, especially when taking into account the inter-person error which can be up to 10%.

In collaboration with the Faculty of Health Studies, University of Ljubljana, we continued the work on the Wartenberg pendulum test where a 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 synovial fluid and to detect anomalies. Several groups of people were tested, belonging to different age populations and some of them being affected by diabetes.

In collaboration with the Paediatric Clinic at the University Medical Centre Ljubljana and the Biotechnical Faculty, the University of Ljubljana,

we performed a clinical trial on the usefulness of Open Platform for Clinical Nutrition (http://opkp.si). The study involved 50 pregnant women and nursing mothers, who logged a four-day food diary through the OPKP. We analyzed the accuracy of the calculation of energy and nutrition logs for all the nutrients that are essential for pregnant women and nursing mothers. The calculated values were compared with the analytical values. The study results are crucial for the continuation of the work in this area.

We were developing a wireless kitchen scale that informs diabetic patients about the carbohydrate content of food in real time. The scale is wireless and connected to a mobile phone or a computer that has an Internet access and runs the OPKP. This embedded system may also be used by other patients with special nutritional needs, as well as by researchers (e.g., in space research).

Within the European project EuroFIR NEXUS we have participated in the program modelling, implementation and testing of an information platform that integrates the information systems of 50 EuroFIR Member States.

In December 2011, we successfully completed a bilateral project with the University of Pecs in Hungary. In

In industrial project with ETA Cerkno d.o.o. we have made an application for the efficient planning of the production of cooking plates, where we increased the theoretical efficiency of the production lines to 99%. completed a blateral project with the University of Pecs in Hungary. In collaboration with the Information Systems Department, we upgraded the Open Platform for Clinical Nutrition (http://opkp.si) with an English user interface and a knowledge database of nutritional recommendations and guidelines for selected target populations. The knowledge base is an important source of information and data needed for an automatic generation of diets for patients with special nutritional needs.

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 dedicated to the stochastic optimization techniques.

### Some outstanding publications in the past three years

- 1. B. Koroušić Seljak. Computer-based dietary menu planning. J. Food Compos. Anal., 2009, vol. 22, no. 5, pp. 414-420.
- 2. K. Tashkova, P. Korošec, J. Šilc, L. Todorovski, S. Džeroski. Parameter estimation with bio-inspired meta-heuristic optimization: modelling the dynamics of endocytosis. BMC Syst. Biol., 2011, vol. 5, pp. 159.
- 3. D. Torkar, B. Zmazek, J. Voupotič, I. Kobal. Application of artificial neural networks in simulating radon levels in soil gas. Chem. Geol., 2010, vol. 270, no. 1/4, pp. 1-8.
- 4. R. Pačnik, F. Novak. A high-sensitivity hydraulic load cell for small kitchen appliances. Sensors, 2010, vol. 10, no. 9, pp. 8452-8465.
- 5. G. Papa, V. Vukašinović, P. Korošec. Guided restarting local search for production planning. Eng. Appl. Artif. Intell., [in press 2011].

### Organization of conferences, congress and meetings

1. AVN, The 18th workshop Nature-Inspired Algorithms, 13 September 2011, Ljubljana, Slovenia

# INTERNATIONAL PROJECTS

- 1. The EuroFIR Food Platform: Further Integration, Refinement and Exploitation of for its Long term Self-sustainability EuroFIR NEXUS
  - 7 FP
  - MOU, 265967

EC; Mary Anderson, Institute of Food Research, Norwich, Great Britain; Paul Finglas, EuroFIR AISBL, Brussels, Belgium

- Asst. Prof. Barbara Koroušić Seljak
- Enhancing Lifelong Learning for the Electrical and Information Engineering Community ELLEIEC Surveyor
  - ERASMUS

2008-3199/001-001, 142814-LPP-1-2008-FR-ERASMUS-ENV

ECG, M. Hamed Yahoui, L'Université Claude Bernard Lyon 1, Villeurbanne Cedex, France Prof. Franc Novak

High-Performance Computer-Based Dietary Menu Planning

BI-HU/10-11-015

Asst. Prof. Istvan Vassanyi, University of Pannonia, Dept. of Information Systems, Veszprem, Hungary Asst. Prof. Barbara Koroušić Seljak

# **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

# RESEARCH PROGRAM

1. Computing structures and systems Prof. Franc Novak

# NEW CONTRACTS

- 1. Cooperation within the RR3 Energy efficient refrigerator Gorenje Gospodinjski Aparati,d.d. Asst. Prof. Gregor Papa
- Eating for two healthy eating and exercise from conception onwards Ministry of Health Republic of Slovenia Asst. Prof. Barbara Koroušić Seljak

# MENTORING

### Ph. D. Theses

- 1. Roman Pačnik, Hydraulic load cells for measurement of small loads (mentor Franc Novak; co-mentor Marija Kosec).
- Denis Špelič, Lossless compression of segmented voxel data (mentor Borut Žalik; comentor Franc Novak).

### M. Sc. Thesis

1. Andrej Jerman Blažič, Educational web applications in vocational education and training in Slovenia (mentor Franc Novak).

# VISITORS FROM ABROAD

 Asst. Prof. István Vassányi, Balázs Gaál, M.Sc. and Balázs Pintér, BSc, University of Pannonia, Department of Information Systems, Veszprém, Hungary, 17–24 October 2011

## STAFF

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- Asst. Prof. Barbara Koroušić Seljak
   Prof. Franc Novak, Head
- Prof. Franc Novak, Head
   Asst. Prof. Gregor Papa
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- Postdoctorial associates
- 7. Dr. Uroš Kač\*, left 03.02.11
- 8. Dr. Drago Torkar
- Postgraduates
- 9. Lucas Benedičič\*\*

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 Uroš Legat, B. Sc.
 *Katerina Tashkova, B. Sc., left 01.07.11* Vida Vukašinović, B. Sc.
 Technical and administrative staff
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Note: \* part-time JSI member \*\* postgraduate financed by industry

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## 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 of knowledge technologies include intelligent data analysis (machine learning, data mining, and knowledge discovery in databases), semantic data mining and semantic web, language technologies and computational linguistics, decision support and knowledge management. In addition to knowledge technologies research, we also develop applications in environmental sciences and ecology, medicine and health care, biomedicine and bioinformatics, economy and marketing.

In 2011 we were involved in 11 national and 12 European projects, most of them founded by the seventh framework programme (7FP). In terms of our collaboration in the EU projects, we are the most successful programme group in Slovenia.

In the area of intelligent data analysis and data mining we have developed several new methods. (a) The Head: new approach for creating and implementing data mining workflows in our service-oriented knowledge discovery Prof. Nada Lavrač platform Orange4WS was published in the Computer Journal. (b) We implemented the SegMine methodology in the Orange4WS platform that, together with the BioMine system for detection of new links between genes, allows a semantic gene expression analysis by using bio-ontologies as background knowledge; this work was published in the BMC Bioinformatics journal. (c) We have developed a new system for bisociative knowledge discovery

called CrossBee for discovering new connections between different medical domains. (d) We have developed new methods for learning regression trees that take into account spatial or network autocorrelation in the values of the target variable. (e) We have developed new methods for learning from data streams, in particular the methods for learning different kinds of

ensembles (including the option trees for regression). (f) We have developed new methods for structured output prediction, based on the nearest-neighbour principle. We have successfully concluded our work in the 7FP project

BISON (Bisociation Networks for Creative Information Discovery), where we developed the methods for discovering bisociative links between different contexts and domains. We have collaborated in the 7FP 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 a subgroup discovery and co-organized a successful Videolectures.net Challenge aimed at developing improved recommendation system for video lectures. We continued successful collaboration within the 7FP project PHAGOSYS (Systems biology of phagosome formation and maturation - modulation by intracellular pathogens), where the emphasis was on the use of meta-heuristic methods for parameter estimation in models of dynamic systems, in particular for the task of modelling endocytosis, an important process of immune response. We became partners in two new 7FP projects: SUMO (Supermodelling by combining imperfect models) and REWIRE (Rehabilitative Wayout In Responsive home Environments). The Figure 1: CrossBee is a web application that implements an algorithm SUMO project deals with the problem of learning supermodels (ensemble models of dynamic systems that combine the existing models), and with the use of supermodels in climate modelling. The REWIRE project focuses on the

development of a new approach to rehabilitation, which uses virtual-reality-based games for rehabilitation at home and wearable sensors (as well as machine learning) to monitor and adaptively plan rehabilitation. In the area of text and web mining and heterogeneous information

networks analysis we participated in three European projects: FIRST (large scale information extraction and integration infrastructure for supporting financial decision making), ENVISION (ENVIronmental Services Infrastructure with ONtologies), and FOC (Forecasting Financial Crises). We are one of

## We successfully organized the "13th Conference

B-Term Identify (Analysis

for discovering hidden links in literatures from different scientific domains. It provides the user with a list of key terms (shown in the figure) which have the potential for cross-domain scientific discovery.

on Artificial Intelligence in Medicine" (AIME 2011) in Bled, Slovenia.



Tomaž Erjavec, together with Matija Ogrin from ZRC SAZU, again received the Google Digital Humanities Research Award for his work on language models for historical Slovene.





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[7]	, pobožnim srcem in vestjo pridnost in	ljubezen	k svojemu stanu združi , se bo
[8]	mulhtre nove forte podati . S polebno	ljubesnijo	sa isobrashenje rokođelikiga ftanu v rifanju fta
	muštre nove sorte podati , s posebno	ljubeznijo	za izobraženje rokođelskega stanu v risanju sta
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[10]	ponudilh . Ti fi shiva podoba nar_ferzhnejlhi	ljubesni	, ker fvojiga blishniga , bodi_fi kdorkolj
	ponudiš . ti si živa podoba najsrečnejše	ljubezni	, ker svojega bližnjega , bodisi kdorkoli
[11]	fvojiga blishniga, bodi_fi kdorkolj, v	ljubesni	s rozhizami objameľh, in ga fvoje
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[12]	terdóbo ferzá , ga ogreje in odpira	ljubesni	, pogafi fhe zlo hude fovrafhtva in
	trdobo srca , ga ogreje in odpira	ljubezni	, pogasi še celo huda sovraštva in
1131	— Prijatel ! kteri le eno ifkro	ljubesni	do zhbeliz imalh , — in kdo
	— prijatelj ! kateri le eno iskro	ljubezni	do čebelic imaš , — in kdo
[14]	je kje negodno zaljubil , in nedosegliva	ljubezen	mu žalostno serce napravlja ; de je
	je kje negodno zaljubil , in nedosegljiva	ljubezen	mu žalostno srce napravlja ; da je
[15]	življenju boljimu , Slovó je kratko za	ljubezen	dolgo ! ( Odide . ) Dünoa
	življenju boljšemu , slovo je kratko za	liubezen	dolgo ! ( odide . ) dünoa

Figure 2: Concordances over a corpus of historical Slovene with modernised forms of words. The corpus and associated programs have been developed in the scope of the EU project IMPACT and the Google Award "Developing language models for historical Slovene".

the key partners in the 7FP project FIRST where we focus on analyzing large amounts of dynamic and heterogeneous sources of financial information. The daily work and the business success of all decision makers in this industry depend on the availability of such highly trustable, easily acquirable information. Our focus in this project is online data mining (financial news, blogs and tweets) in near-real time over vast amounts of constantly evolving data. In 2011 we designed the architecture and implemented a software system for capturing and annotating online texts in real time. We daily monitor 200 financial web sources and capture about 40,000 pieces of news per day. In the future we will focus on data analysis and solving practical problems for end users (financial-product sentiment analysis, analysis of financial institutions' reputation, online deceit detection). In the ENVISION project we developed a methodology to support the semantic description of geographic data and services. We specifically focused on supporting multilinguality in ontology management that enables end users to search for the basic building blocks of semantic descriptions. This methodology was implemented as a web application and will represent one of the modules of the on-line

environmental decision support portal. In September 2011 we started working on the7FP project FOC that focuses on forecasting financial crises. Our role in this project is to analyze non-financial crisis indicators based on the sentiment analysis of large streams of textual data.

### Elena Ikonomovska received Best Submission Award at the doctoral symposium of the EDBT/ **ICDT 2011 Joint Conference.**

In the area of language technologies we applied the methodology developed for contemporary Slovene to the development of annotated corpora, computational lexica and an annotation tool for historical Slovene. These resources are important for a better accessibility of the Slovenian written cultural heritage on the dLib.si digital library portal of the National

and University Library of Slovenia (NUL), as well as for enabling empirically supported diachronic studies of the Slovene language. The work on the development of the language resources for historical Slovene was undertaken within the scope of the 7FP project IMPACT (Improving Access to Text), in which we collaborate with the NUL,



Figure 3: Screenshot of a workflow in the Orange4WS environment that implements the SegMine methodology. SegMine enables the construction of new biological hypotheses by linking the results of a semantic analysis of experimental microarray data to the knowledge available in the public biological databases.

historical Slovene", in which we collaborate with the Scientific Research Centre of the Slovenian Academy of Sciences and Arts (SRC SASA). In the scope of the national project "Unknown 17th and 18th century manuscripts of Slovenian literature: information-technology aided register, scholarly editions and analyses", we continued joint work with SRC SASA on complex digital editions of older Slovenian literature, where we implemented a Fedora Commons platform for manuscript viewing and searching. The platform was also used to host a digital edition of the Slovenian Biographic Lexicon, developed by SASA. In the second half of 2011 we also started joint work with SRC SASA on the national project "Leading Slovenian humanists from the 16th to the mid-19th century". We continued work on linguistic annotation of parallel bi-lingual corpora, performed in the scope of the national project "Slovenian translation 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 to be used to enable linguistic studies of translation processes, while also being useful for the development of multilingual language technologies. In cooperation with the same department we also

continued work on enlarging the scope and variety of information in the Slovenian semantic lexicon sloWNet. In the field of access to and standardisation of language resources we worked on the EU project FlareNet "Fostering Language Resources Network". As one of the founding members we joined, at the end of 2010, the COST project

Sašo Džeroski gave an invited lecture at the 9th International Conference on Formal Concept Analysis, held in Nicosia, Cyprus, in May 2011. MUMIA (Multilingual and Multifaceted Interactive Information Access) and the European ESF network NetWordS (The European Network on Word Structure). We intensely collaborated in the work of the Slovenian Institute of Standardisation, as the Slovenian delegates of ISO/TC37/SC4 »Terminology and Other Language and Content Resources/Language Resources Manage-

ment«, by taking part in the meetings of ISO TC 37 and by reviewing, translating and approving Slovenian standards from this field. At the Slovenian Ministry of Culture we are active in the preparation of the National Programme for

the Language Policy 2012-2016, and in taking the steps necessary for Slovenia to join the research infrastructure CLARIN (Common Language Resources and Technology Infrastructure).

In the area of **decision support** our long-term goal is to develop the methods and techniques of decision modelling, support them with software and integrate them with the data mining systems. In 2011 we implemented a Figure 4: Hierarchical annotation of medical images, where a set of method for qualitative multi-attribute decision making DEX on the Decision images is given with their visual descriptors and annotations from a Deck platform. Decision Deck is an open platform that facilitates a uniform incorporation and connection of various multi-attribute modelling methods



hierarchy of labels.

and algorithms. We developed a new version (3.03) of the computer program for multi-attribute decision making DEXi by introducing better facilities for the utility functions' definition and data interchange. We also developed new methods for ranking the alternatives in qualitative multi-attribute models, based on copulas, which improve the sensitivity of decision models and alleviate some drawbacks of the existing methods.

## Some outstanding publications in the last year

- 1. Vid Podpečan, Nada Lavrač, Igor Mozetič, Petra Kralj Novak, Igor Trajkovski, Laura Langohr, Kimmo Kulovesi, Hannu Toivonen, Marko Petek, Helena Motaln, Kristina Gruden. SegMine workflows for semantic microarray data analysis in Orange4WS. BMC Bioinformatics, 2011, vol. 12, no. 416, pp. 1-16, doi: 10.1186/1471-2105-12-416
- 2. Vid Podpečan, Monika Zemenova, Nada Lavrač. Orange4WS environment for service-oriented data mining. The Computer Journal., [in press] 2011, 17 pp., doi:10.1093/comjnl/bxr077.
- 3. Daniela Stojanova, Andrej Kobler, Peter Ogrinc, Bernard Ženko, Sašo Džeroski. Estimating the risk of fire outbreaks in the natural environment. Data Mining and Knowledge Discovery, [in press] 2011, 10 pp., doi: 10.1007/s10618-011-0213-2.
- 4. Tomaž Erjavec. MULTEXT-East : Morphosyntactic resources for Central and Eastern European languages. Language Resources and Evaluation, [in press] 2011, 12 pp., doi: 10.1007/s10579-011-9174-8.
- 5. Ivica Dimitrovski, Dragi Kocev, Suzana Loskovska, Sašo Džeroski. Hier-44, no. 10/11, pp. 2436-2449.

## Organization of conferences, congress and meetings

- 1. Subconference: Intelligent system, Information Systems 2011, Ljubljana, Slovenia, 10-14 Oct. 2011
- 2. 13th Conference on Artificial Intelligence in Medicine AIME'11, Bled, Slovenia, 2-6 Jul. 2011
- Project meeting of European project ENVISION, Kranjska Gora, Slovenia, 25-28 Jan. 2011 3.
- 4. Project meeting of European project FIRST, Bled, Slovenia, 16-18 May 2011

## INTERNATIONAL PROJECTS

1.	Rehabilitative Wayout In Responsive home Environments
	REWIRE
	7 ED 207712

EC; Prof. Alberto Borghese, Universita degli Studi di Milano, Milano, Italy Prof. Sašo Džeroski

- Supermodeling by Combining Imperfect Models Enlarged EU 2.
  - SUMO
  - 7. FP. 266722

EC; Prof. Ljupco Kocarev, Macedonian Academy of Sciences and Arts, Skopje, Macedonia Prof. Sašo Džeroski

- Forecasting Financial Crises Enlarged EU 3. FOC II
  - 7. FP, 255987
  - EC; Dr. Guido Caldarelli, Consiglio Nazionale delle Ricerche, Rome, Italy
  - Dr. Igor Mozetič, Miha Grčar, B. Sc.
- e-Laboratory for Collaborative Interdisciplinary Research in Data Mining and Data 4 Intensive Sciences



Figure 5: Real-time sentiment analysis of financial tweets, performed within project FIRST. In the case of the Netflix stock, the graphs show that archical annotation of medical images. Pattern Recognition, 2011, vol. the sentiment dropped before the big price plunge on 19 September 2011.

5.	e-LICO 7. FP, 257680 EC; Dr. Mélanie Hilario, Universite de Geneve, Carouge, Switzerland Prof. Nada Lavrač, Asst. Prof. Martin Žnidaršič, Mitja Jermol, M. Sc. Large Scale Information Extraction and Integration Infrastructure for Supporting
	Financial Decision Making
	FIRST
	7. FP, 257928
	EC; Tomas Pariente Lobo, Atos Origin Sociedad Anónima Espanola, Madrid, Spain
	Miha Grčar, B. Sc., Prof. Nada Lavrač
5.	Improving Access to Text
	IMPACT
	7. FP, 215064
	EC; Hildelies Balk, Koninklijke Biblioteek, Haag, The Netherlands
	Asst. Prof. Tomaž Erjavec, Jan Jona Javoršek, B. Sc.
7.	Systems Biology of Phagosome Formation and Maturation, Modulation by Intracellul
	Pathogens

8

PHAGOSYS 7. FP, 223451, HEALTH-F4-2008-223451 EC; Dr. Brian D. Robertson, Imperial College London, Centre for Molecular Microbiology and Infection, London, Great Britain Prof. Sašo Džeroski Bisociation Networks for Creative Information Discovery BISON 7. FP, 211898 EC; Prof. Michael Berthold, Universität Konstanz, Konstanz, Germany Prof. Nada Lavrač 1. 9 Environmental Services Infrastructures with Ontologies ENVISION 2 7. FP, 249120 EC; Bjorn Skjellaug, Arne J. Berre, Stiftelsen Sintef, Trondheiim, Norway 3 Miha Grčar, B. Sc., Prof. Nada Lavrač, Prof. Dunja Mladenić, Mitja Jermol, M. Sc. Fostering Language Resources Network 4 FLaReNet e-Contentplus ECP-2007-LANG-617001 EC; Dr. Nicoletta Calzolari, Consiglio Nazionale delle Ricerche (CNR-ILC), Rome, Italy Asst. Prof. Tomaž Erjavec 11. Multilingual and Multifaceted Interactive Information Access MUMIA COST IC1002 EC; Dr. Michail Salampasis, Alexander Technological Educational Institute (T.E.I.) of Thessaloniki, Thessaloniki, Greece Dr. Igor Mozetič, Prof. Nada Lavrač 12. The European Network on Word Structure 9 NetWordŚ RNP Ref. Number 09-RNP-08 ESF; Vito Pirrelli, Institute for Computational Linguistics, Italian National Research Council, Pisa, Italy Asst. Prof. Tomaž Erjavec 13. Google Digital Humanities Research Award Award dtd. 13, 12, 2011 Google Inc, Mountain View, CA, USA Asst. Prof. Tomaž Erjavec Identifying Optimal Management Strategies for Biodiversity and Related Ecosystem 14 Services on Private Forestes BI-US/11-12-048

## MENTORING

## Ph. D. Theses

- Ivica Dimitrovski, Generic system for content based image retrieval (mentor Suzana 1. Loškovska; co-mentor Sašo Džeroski).
- 2 Andrej Kobler, New methods of processing aerial laser scanner data for forest ecosystem monitoring (mentor Krištof Oštir; co-mentor Sašo Džeroski).
- Dragi Kocev, Ensembles for predicting structured outputs (mentor Sašo Džeroski). 3 Viljem Pavlovič, Modelling of alpha-acid content early prediction by hops (Humulus
- lupulus L.) with machine learning models (mentor Črtomir Rozman; co-mentor Marko Bohanec). Aleksander Pur, Model for monitoring and assessment of a public health care network 5
- (mentor Marko Bohanec).

#### M. Sc. Theses

- Robert Čebron, Design of an information system to support education in the secondary 1. school (mentor Bojan Cestnik).
- Vitko Črep, Information system for the management of multi-residential buildings and 2 market opportunities for housing managers (mentor Bojan Cestnik). Silvester Jeršič, The use of UML in procedures of standards ISO 9001 and 14001 (mentor
- 3 Bojan Cestnik).
- Marijan Merljak, Implementing CRM into Business Operations (mentor Bojan Cestnik). 4 Janko Skok, İmpacts of forest management on biodiversity : small mammals in the fir-beech forest of Mt. Snežnik as a model group (mentor Boris Kryštufek; co-mentor 5. Marko Debeliak).
- Li Xiaobin, Implementing DEXi evaluation models in Decision Deck platform (mentor 6. Marko Bohanec).
- Iztok Zajc, Renewal of an information system for logistic support of firefighting 7. interventions (mentor Bojan Cestnik).

#### Bologna M. Sc. Thesis

1. Petra Barber, Use of multi-attribute decision support model in public procurement (mentor Marko Bohanec; co-mentor Ljupčo Todorovski).

Prof. Donald Glenn Hodges, University of Tennessee-Knoxville College of Agricultural Sciences and Natural Resources, Department of Forestry, Wildlife and Fisheries, Knoxville, USA Prof. Marko Debeljak

## **R & D GRANTS AND CONTRACTS**

- Advanced ML methods for automated modeling of dynamic systems Prof. Sašo Džeroski
- Data mining for integrative data analysis in systemic biology Prof. Sašo Džeroski
- Semantic rule discovery in the context of Web services Prof. Nada Lavrač
- Systemic biology approaches to analyzing interactions between pathogens and plants Prof. Nada Lavrad
- Growth and defense trade-offs in multitrophic interaction between potato and its two major pests
  - Prof. Nada Lavrač
- Slovene translation studies resources and research Asst. Prof. Tomaž Erjavec
- The leading humanists in the Slovenian territory between the 16th and mid-19th centuries and their social and cultural environment
- Asst. Prof. Tomaž Erjavec Ecological restoration of natural disturbances in forests Prof. Marko Debeljak
- Unknown 17th and 18th century manuscripts of Slovenian literature: informationtechnology aided register, scholarly editions and analyses Asst. Prof. Tomaž Eriavec
- Analysis and Scenario of Development and Exploration of Forests in Slovenia Prof. Marko Debeljak

## RESEARCH PROGRAM

1 Knowledge Technologies Prof. Nada Lavrač

## VISITORS FROM ABROAD

- 1. Martin Saveski, Skopje, Macedonija, 1 Jan.-1 Nov. 2011
- 2. Dr. Michelangelo Ceci, Dipartimento di Informatica, Universita degli Studi di Bari, Bari, Italy, 9 Jan.-4 Apr. 2011
- Prof. Dr. Don Hodges, Univerza v Tennesseeju, Institute of Agroculture, Knoxwille, USA, 3. 15 Jan.-1 Jul. 2011
- 4. Mag. Ivica Dimitrovski, Faculty of Electrical Engineering and Information Technologies, University Ss. Cyril and Methodius, Skopje, Macedonia, 16.-23. 4. 2011 in 9.-31. 1. 2011
- Jovan Tanevski, University Ss. Cyril and Methodius, Skopje, Makeconia, 5. 3.-3. 4. 2011
- Dr. Werner Dubitsky, University of Ulster, Coleranine, Ireland, 31 Mar.–1 Apr. 2012 6.
- Oliver Schmidt, University of Ulster, Coleranine, Ireland, 31 Mar.-1 Apr. 2012 7.
- Dr. Cesare Furlanello, Fodacione Bruno Kessler, Trento, Italy, 16-23 Apr. 2011 8.
- Dr. Christopher Barnes, Imperial College London, London, Great Britain, 19-22 Jun. 2011 Dr. Boris Delibašić, University of Belgrade, Faculty of Organizational Sciences, Beograd, 10.
- Republic of Serbia, 6-8 Jul. 2011 Dr. Miloš Jovanović, University of Belgrade, Faculty of Organizational Sciences, Beograd, Republic of Serbia, 6-8 Jul. 2011
- Dr. Milan Vukičević, University of Belgrade, Faculty of Organizational Sciences, 12. Beograd, Republic of Serbia, 6-8 Jul. 2011
- 13. Prof. Dr. Barry Hardy, Douglas Connect, Zeiningen, Switzerland, 29.-31. 8. 2011
- Prof. Dr. Joost Kok, Leiden Institute of Advanced Computer Science, Leiden University, 14. Leiden, Netherlands, 11-13 Sept. 2011
- 15. Dr. William Klement, Ottawa-Carleton Institute for Computer Science, School of Electrical Engineering and Computer Science, University of Ottawa, Ottawa, Ontario, Canada, 26-30 Sept. 2011
- Dr. Richard Wheeler, University of Edinburgh, Edinburgh, Scotland, 23 May–12 Jun. 2011 and 10-17 Oct. 2011
- 17 Dr. Gregory Duane, Macedonian Academy of Science and Arts, Skopje, Macedonia, 26 Oct. 2011
- Dr. Stijn Meganck, The Institute for the encouragement of Scientific Research and 18. Innovation, Vrije Universiteit, Brussels, Belgium, 30 Nov.-1 Dec. 2011
- 19. Dr. Taminau Jonatan, The Institute for the encouragement of Scientific Research and Innovation, Brussels, Belgium, 30 Nov.-1 Dec. 2011
- 20. Dr. Dragan Gamberger, Institut Rudjer Bošković, Zagreb, Croatia, 30 Nov. 2011
- 21. Dr. Larisa Soldatova, Aberystwyth University, Department of Computer Science, Aberystwyth, Great Britain, 2-17 Dec. 2011

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- 17. Matjaž Juršič, B. Sc.

## BIBLIOGRAPHY

## **ORIGINAL ARTICLES**

- Nataša Atanasova, Sašo Džeroski, Boris Kompare, Ljupčo Todorovski, Gideon Gal, "Automated discovery of a model for dinoflagellate dynamics", *Environ. model. softw.*, vol. 26, no. 5, pp. 658-668, 2011.
- Jérome Cortet, Dragi Kocev, Caroline Ducobu, Sašo Džeroski, Marko Debeljak, Christophe Schwartz, "Using data mining to predict soil quality after application of biosolids in agriculture", *J. environ. qual.*, vol. 40, no. 6, pp. 1972-1982, 2011.
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- Elena Ikonomovska, João Gama, Sašo Džeroski, "Learning model trees from evolving data streams", *Data mining and knowledge discovery*, vol. 23, no. 1, pp. 128-168, 2011.
- 5. Reuben P. Keller, Dragi Kocev, Sašo Džeroski, "Trait-based risk assessment for invasive species: high performance across diverse taxonomic groups, geographic ranges and machine learning/statistical tools", *Divers. distrib.*, vol. 17, no. 3, pp. 451-461, 2011.
- Lado Kutnar, Andrej Kobler, Sašo Džeroski, "Kakšni bi lahko bili učinki segrevanja ozračja na bukove gozdove v prihodnosti", *Les (Ljublj.)*, let. 63, no. 5, pp. 203-207, 2011.
- Nada Lavrač, Anže Vavpetič, Larisa N. Soldatova, Igor Trajkovski, Petra Kralj Novak, "Using ontologies in semantic data mining with SEGS and g-SEGS", In: Discovery science: 14th International Conference, Ds 2011, Espoo, Finland: proceedings, *Lect. notes comput. sci.*, vol. 6926, pp. 165-178, 2011.
- Nikola Ljubešić, Tomaž Erjavec, "hrWac and siWac: compiling web corpora for Croatian and Slovene", In: Text, speech and dialogue: proceedings, *Lect. notes comput. sci.*, vol. 6836, pp. 395-402, 2011.
- Marta Macedoni-Lukšič, Ingrid Petrič, Bojan Cestnik, Tanja Urbančič, "Developing a deeper understanding of autism: connecting knowledge through literature mining", *autism res. treat.*, vol. 2011, 8 pp., 2011.
- 10. Martin Pavlovič *et al.* (6 authors), "Development of DEX-HOP multiattribute decision model for preliminary hop hybrids assessment", *Comput. electron. agric.*, vol. 75, no. 1, pp. 181-189, 2011.
- 11. Vid Podpečan, Nada Lavrač, Igor Mozetič, Petra Kralj Novak, Igor Trajkovski, Laura Langohr, Kimmo Kulovesi, Hannu Toivonen, Marko Petek, Helena Motaln, Kristina Gruden, "SegMine workflows for semantic microarray data analysis in Orange4WS", *BMC bioinformatics*, vol. 12, no. 416, pp. 416-1-416-16, 2011.
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- 14. Daniela Stojanova, Michelangelo Ceci, Annalisa Appice, Sašo Džeroski, "Network regression with predictive clustering trees", In: Machine learning and knowledge discovery in databases. Part III: European Conference, ECML PKDD 2011, Athens, Greece, *Lect. notes comput. sci.*, vol. 6913, pp. 333-348, 2011.
- Daniela Stojanova, Michelangelo Ceci, Annalisa Appice, Donato Malerba, Sašo Džeroski, "Global and local spatial autocorrelation in predictive clustering trees", In: Discovery science: 14th International Conference, Ds 2011, Espoo, Finland: proceedings, *Lect. notes comput. sci.*, vol. 6926, pp. 307-322, 2011.
- 16. Katerina Taškova, Peter Korošec, Jurij Šilc, Ljupčo Todorovski, Sašo Džeroski, "Parameter estimation with bio-inspired meta-heuristic optimization: modeling the dynamics of endocytosis", *BMC systems biology*, vol. 5, pp. 159-1-159-52, 2011.
- 17. Aneta Trajanov, "Analysis of results of ecological simulation models with machine learning", *Informatica (Ljublj.)*, vol. 35, no. 2, pp. 285-286, 2011.
- Monika Žáková, Petr Křemen, Filip Železný, Nada Lavrač, "Automating knowledge discovery workflow composition through ontology-based planning", *IEEE trans. autom. sci. eng.*, vol. 8, no. 2, pp. 253-264, 2011.

## **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

- 1. Marko Debeljak, Sašo Džeroski, "Decision trees in ecological modelling", In: *Modeling complex ecological dynamics: an introduction into ecological modelling for students, teachers & scientists*, Fred Jopp, ed., Berlin, Heidelberg [etc.], Springer, cop. 2011, pp. 197-209.
- Tomaž Erjavec, "Slovenska prevodna književnost 1848-1918: digitalna knjižnica in korpus AHLIB", In: *Meddisciplinarnost v slovenistiki*, (Obdobja, Simpozij, = Symposium, 30), Simona Kranjc, ed., 1. natis, Ljubljana, Znanstvena založba Filozofske fakultete, 2011, pp. 33-40.
- Tomaž Erjavec, Jan Jona Javoršek, Matija Ogrin, Petra Vide Ogrin, "Od biografskega leksikona do znanstvenokritične izdaje: vprašanje trajnosti elektronskih besedil", *Knjižnica (Tisk. izd.)*, vol. 55, no. 1, pp. 103-114, 2011.
- Tomaž Erjavec, Ines Jerele, Maša Kodrič, "Izdelava korpusa starejših slovenskih besedil v okviru projekta IMPACT", In: *Meddisciplinarnost v slovenistiki*, (Obdobja, Simpozij, = Symposium, 30), Simona Kranjc, ed., 1. natis, Ljubljana, Znanstvena založba Filozofske fakultete, 2011, pp. 41-47.
- 5. Petra Kralj Novak, Nada Lavrač, Geoffrey I. Webb, "Supervised descriptive rule induction", In: *Encyclopedia of machine learning: with 293 figures and 78 tables*, Claude Sammut, ed., Geoffrey I. Webb, ed., New York, Springer, 2011, pp. 938-941.

- 6. Matija Ogrin, Jan Jona Javoršek, Tomaž Erjavec, "Rokopisi slovenskega slovstva baročne in razsvetljenske dobe: predmet več ved in metod", In: *Meddisciplinarnost v slovenistiki*, (Obdobja, Simpozij, = Symposium, 30), Simona Kranjc, ed., 1. natis, Ljubljana, Znanstvena založba Filozofske fakultete, 2011, pp. 337-341.
- 7. Ingrid Petrič, Tanja Urbančič, Bojan Cestnik, "Ontological representation of virtual business communities: how to find right business partners", In: *Innovations in smes and conducting e-business: technologies, trends and solutions*, (Premier reference source), Maria Manuela Cruz-Cunha, ed., Joao Varajao, ed., Hershey, New York, London, Information Science Reference, Igi Global, 2011, pp. 263-277.

## PUBLISHED CONFERENCE PAPERS

## **Invited Papers**

- Marko Debeljak, "Gozdovi v svetu in Sloveniji", In: *Povezanost procesov: zbornik prispevkov: proceedings*, Mednarodni posvet Biološka znanost in družba, Ljubljana, 6. in 7. oktober 2011 = Conference on Bioscience and Society, October 6-7, 2010, Ljubljana, Slovenia, Minka Vičar, ed., Saša Kregar, ed., Frances M. Ashcroft, 1. izd., Ljubljana, Zavod RS za šolstvo, 2011, pp. 86-94.
- Sašo Džeroski, "Inductive databases and constraint-based data mining", In: *Formal concept analysis: proceedings*, (Lecture note in computer science, Lecture notes in artificial intelligence, vol. 6628), 9th International Conference, ICFCA 2011, May 2-6, 2011, Nicosia, Cyprus, Petko Valtchev, ed., Robert Jäschke, ed., Heidelberg [etc.], Springer, cop. 2011, pp. 1-17.

## **Regular** papers

- 1. Maja Bračič Lotrič, Bojan Cestnik, "Literature mining of blood flow regulatory mechanisms for finding cross context relations", In: *Computer systems and technology: 12th International Conference, CompSysTech'11, June 16-17, 2011, Vienna, Austria: proceedings*, (ACM international conference proceedings series, vol. 578), Boris Rachev, ed., Angel Smrikarov, ed., New York, ACM, = Association for Computing Machinery, 2011, pp. 353-358.
- Bojan Cestnik, Tanja Urbančič, Ingrid Petrič, "Ontological representations for supporting learning in business communities", In: *e-Learning'11: proceedigs of the International Conference on e-Learning and the Knowledge Society, 25-26 August 2011, Bucharest, Romania,* Angel Smrikarov, ed., Bucharest, ASE Publishing House, 2011, pp. 260-265.
- 3. Christian Chiarcos, Tomaž Erjavec, "OWL/DL formalization of the MULTEXT-East morphosyntactic specifications", In: *LAW V*, 5th Linguistic Annotation Workshop, June 23, 2011, Portland, Oregon, Portland, Association for Computational Linguistics, 2011, pp. 11-20.
- 4. Marko Debeljak, Bernard Ženko, Aleš Poljanec, "Napovedni modeli razvoja gozdov v Sloveniji", In: *Priprava gozdnogospodarskih in lovsko upravljalskih načrtov območij za obdobje 2011-2020: zbornik prispevkov*, (Gospodarjenje z gozdovi in načrtovanje, 5), Andrej Bončina, ed., Ljubljana, Oddelek za gozdarstvo in obnovljive gozdne vire - Biotehniška fakulteta, 2011, pp. 11-14.
- 5. Marko Debeljak, Bernard Ženko, Aleš Poljanec, "Predictive models of forest development in Slovenia", In: *Innovations in sharing environmental observations and informations: proceedings of the 25th EnviroInfo International Conference, October 5-7, 2011, Ispra, Italy,* Werner Pillmann, ed., S. Schade, ed., Paul Smits, ed., Aachen, Shaker Verlag, cop. 2011, pp. 97-100.
- 6. Tomaž Erjavec, "Automatic linguistic annotation of historical language: ToTrTaLe and XIX century Slovene", In: *LaTeCH 2011*, 5th Workshop on Language Technology for Cultural Heritage, Social Sciences, and Humanities [and] 49th Annual Meeting of the Association for Computational Linguistics: human language technologies (ACL/HLT), June 19-24, 2011, Portland, Oregon, USA, Kalliopi Zervanou, ed., Piroska Lendvai, ed., Portland, Association for Computational Linguistics, 2011, pp. 33-38.
- Tomaž Erjavec, Christoph Ringlstetter, Maja Žorga Dulmin, Annette Gotscharek, "A lexicon for processing archaic language: the case of XIXth century Slovene", In: *An ESSLLI 2011 Workshop*, First International Workshop on Lexical Resources, An ESSLLI 2011 Workshop, Ljubljana, Slovenia - August 1-5, 2011, [S. l., s. n., 2011], pp. 24-30.
- Valentin Gjorgjioski, Dragi Kocev, Sašo Džeroski, "Comparison of distances for multi-label classification with PCTs", In: Zbornik 14. mednarodne multikonference Informacijska družba - IS 2011, 10.-14.

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- 9. Elena Ikonomovska, "Regression on evolving multi-relational data streams", In: *Electronic conference proceedings*, Uppsala, ACM, 2011, 7 pp.
- Elena Ikonomovska, João Gama, Sašo Džeroski, "Incremental multitarget model trees for data streams", In: Proceedings of the 26th Annual ACM Symposium on Applied Computing 2011, Taichung, Taiwan, March 21 - 24, 2011, [S. l.], ACM, cop. 2011, pp. 988-993.
- 11. Elena Ikonomovska, João Gama, Bernard Ženko, Sašo Džeroski, "Speeding up Hoeffding-based regression trees with options: a", In: *Proceedings of the Twenty-eighth International Conference on Machine Learning: [Bellevue, Washington, USA, June 28 - July 2, 2011]*, Lise Getoor, ed., Tobias Scheffer, ed., [Madison, International Machine Learning Society], 2011, pp. 537-552.
- 12. Stojan Košti, Bojan Cestnik, "Using business analysis to select appropriate e-learning system", In: *e-Learning'11: proceedigs of the International Conference on e-Learning and the Knowledge Society, 25-*26 August 2011, Bucharest, Romania, Angel Smrikarov, ed., Bucharest, ASE Publishing House, 2011, pp. 165-176.
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- 14. Borut Sluban, Dragan Gamberger, Nada Lavrač, "Performance analysis of class noise detection algorithms", In: *Stairs 2010: proceedings of the Fifth Starting Al Researchers' Symposium in conjunction with the 19th European Conference on Artificial Intelligence (ECAI 2010), 16-20 August 2010, Lisbon, Portugal*, (Frontiers in artificial intelligence and applications, vol. 222), Thomas Ågotnes, ed., Amsterdam ... [et al.], IOS Press, pp. 303-314.
- 15. Borut Sluban, Matjaž Juršič, Bojan Cestnik, Nada Lavrač, "Evaluating outliers for cross-context link discovery", In: Artificial intelligence in medicine: proceedings, (Lecture notes in computer science, Lecture notes in artificial intelligence, 6747), 13th Conference on Artificial Intelligence in Medicine, AIME 2011, Bled, Slovenia, July 2-6, 2011, Mor Peleg, ed., Nada Lavrač, ed., Carlo Combi, ed., Berlin [etc.], Springer, cop. 2011, pp. 343-347.
- 16. Jasmina Smailović, Martin Žnidaršič, Miha Grčar, "Web-based experimental platform for sentiment analysis", In: *The proceedings of the 3nd International Conference on Information Society and Information Technologies - ISIT 2011, [Dolenjske Toplice, 9-11 November 2011]*, Matej Mertik, ed., Novo mesto, Faculty of Information Studies, 2011, 6 pp.
- Anže Vavpetič, Igor Trajkovski, Petra Kralj Novak, Nada Lavrač, "Semantic data mining system g-SEGS", In: *PlanSoKD'11, Planning to Learn and Service-Oriented Knowledge Discovery September 9, 2011, Athens, Greece,* Jörg-Uwe Kietz, ed., Simon Fischer, ed., Nada Lavrač, ed., Vid Podpečan, ed., [S. l., s. n.], 2011, pp. 17-29.

## **RESEARCH MONOGRAPH**

1. Aneta Trajanov, Machine learning in agroecology: from simulation models to co-existence rules, Saarbrücken, LAP Lambert, cop. 2011.

## THESES

#### Ph. D. Thesis

1. Dragi Kocev, *Ensembles for predicting structured outputs:* doctoral dissertation, Ljubljana, [D. Kocev], 2011.

### B. Sc. Theses

- 1. Nejc Trdin, Decision support model for management of water sources: undergraduate thesis, Ljubljana, [N. Trdin], 2011.
- 2. Anže Vavpetič, The use of ontologies as background knowledge in data mining: undergraduate thesis, Ljubljana, [A. Vavpetič], 2011.

## 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 modelling, 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. Dr. Ivan Bratko.

Intelligent systems simulate intelligence so that a typical user perceives them as truly intelligent. In reality, these systems use complex mechanisms implementing them on digital computers to imitate human behaviour as well as exploiting raw, exponentially growing computer power.



E-C

Ambient intelligence is an increasingly relevant research area. It aims at introducing the technology into our everyday environment in a friendly way, undemanding for the user. Considering the rapid aging of the population, Head: one of the area's main goals is the care for the elderly. We addressed it in the EU 7FP project Confidence, which Prof. Matjaž Gams successfully ended in 2011. Within this project an intelligent home-care system was developed, with the goal of prolonging the independence of the elderly. This was achieved by recognising the falls and other health problems from the sensor data. Last year we focused on long-term health problems. In addition, we compared radio sensors for determining the locations of the user's body parts, and accelerometers. This research was extended outside

the project with a thorough study of the effects of the sensor placement and the type (location/acceleration) on the activity and fall recognition. Furthermore we also looked at the analysis of human movement for the purpose of recognising health problems, such as a leg pain and Parkinson's disease. In the European project CHIRON we worked on monitoring chronic heart-disease patients at home. Our task is the activity recognition and an estimation of the patient's energy expenditure with accelerometers. This information represents the basis for observing the patient's heartbeat using ECG. Additionally, we worked on a decision-support system for physicians. Its main task was an assessment of the risk to the patient's health. To this end we developed two methods: the first assesses the risk on the basis of the expert knowledge about the parameters monitored in the project, while the second detects deviations from a patient's normal condition. In the ELKOV22 project we cooperated with the Elgoline, Kovinoplastika and INTECH-LES razvojni center companies to develop an intelligent door system. Such a door uses sensors to detect opening, closing and violent actions. This makes it possible to react to unusual and dangerous events, and to generally increase security.



Figure 1: Human activity recognition and energy expenditure estimation with accelerometers in the Chiron project

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 the evolutionary computation methods. We study extensions of evolutionary

algorithms for a multiobjective optimization and their parallelization, and apply these algorithms in engineering design and optimization problems. Specifically, we are developing a method for visualization of multidimensional fronts of nondominated solutions in an multiobjective optimization, and an algorithm for discovering the optimal car-driving strategies with respect to the travelling time and the fuel consumption. In addition, our

In the European project CHIRON we monitor chronic heart-disease patients at home. The recognized patient's activity and the estimated energy expenditure represent the context for the observation of the patient's heartbeat.

work is motivated by the optimization of metallurgical production processes that is a subject of two research projects carried out together with the University of Nova Gorica, the 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 the partners from five European countries, we carry out the EU 7FP project MIRABEL (originally called MIRACLE). Its goal is to develop a computer infrastructure to efficiently balance between the generation and consumption of electrical energy using an increased amount of energy from renewable sources. This infrastructure relies on flex-



Figure 2: Discovered behaviour pattern with the corresponding symbolic description in the form of IF-THEN rules.

In the ELKOV22 project we cooperate with industrial partners to develop an intelligent door system. The project is focused on security and thedetection of unusual events during an entrance.

ible offers for energy generation and consumption, their aggregation and scheduling. For this project we implemented scheduling algorithms that assign time and energy amount to the relevant offers. For the Restoration Center, Ljubljana, which is part of the Institute for the Protection of Cultural Heritage of Slovenia, we continued to develop Pedius, an innovative software tool to support the restoration of wall paintings.

In the field of agent modelling we are focused on the behaviour analysis of individuals and groups. Most of the work is performed for the EUSAS project, which is funded by the European Defence Agency. The scope of this project is to develop methods for multi-agent modelling of asymmetric conflicts. The aim is to develop a new approach to mission analysis and training for low level units facing asymmetric threats in an urban environment. The developed tool can be used to discover the common agent strategy by knowing only the low-level agent behaviour 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, the objective is to transfer some of the observed behaviour patterns into highly realistic and reusable models of human behaviour in riots. We also studied the behaviour of individuals, trying to detect suspicious behaviour at the airport. The goal is to detect suspicious behaviour from a sequence of events, even though no single event on its

own can indicate that certain behaviour is suspicious. Individual events are recognized from multiagent interactions. Whether a sequence of such events is suspicious is established using a probabilistic Bayesian framework. We showed that an optimum evaluation of suspiciousness is not feasible in practice. Instead, we proposed a naïve and



Figure 3: Computer supported restoration of wall paintings with the Pedius program

develop a computer infrastructure to efficiently

electrical energy using an increased amount of

balance the generation and consumption of

energy from renewable sources.

a heuristic approach and tested them on a simulated airport domain. The heuristic approach achieved high performance resulting in a high-detection rate and low false-alarm ratio. In the field of speech and language technologies we work on speech

synthesis, forensic speaker recognition, semantic analysis of texts and question answering. Together with the Amebis company, we developed a new speech synthesizer for Slovene. In cooperation with the national television and radio, RTV Slovenia, we developed a phonetically rich and balanced speech database for a corpus-based speech synthesis. In speaker recognition we investigated the correlation between the speech quality in telephony and the performance of automatic-speaker verification. In question answering, a machine-learning classifier that classifies questions by expected answer type was developed. We developed a new version of the virtual assistant, which uses state-of-the-art web technology to improve the user experience.

Robi, the Institute's virtual assistant, received some handy new functions, for example, the ability to search the employees' contact data. We deployed the Little Dragon that answers questions of the visitors to the Municipality

of Ljubljana website (http://www.ljubljana.si/si/mol/). We also developed an assistant to be used in an intelligent home.

The department received two major awards in 2011. At the Third Industrial Forum of Innovation, R&D and Technology, we received the Taras Award for a successful collaboration between a research institution and industry. It was awarded to the iLab project carried out in collaboration with the Lotrič company. In the project a system for monitoring the conditions in

a laboratory was developed. At the Sixth Slovenian Innovation Forum we received the Silver Award for excellence in innovative industries for the Pedius system. The system provides computer support for the restoration of wall paintings from plaster fragments.

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.

From 10 to 14 October 2011, the 14th international multiconference Information Society (IS 2011) took place at the Jožef Stefan Institute. It consisted of nine independent conferences with 193 papers, contributed by 299 (co) authors from 13 countries. Four conference awards were given. Two were traditional: for exceptional contribution to the development and promotion of the information society, and for the current achievements in the field of

## The goal of the 7FP project MIRABEL is to

information society. Two, however, were new: the information strawberry and lemon for the best and worst public information-society services, respectively.

## Outstanding publications in the last year

- Kaluža Boštjan, Dovgan Erik, Tušar Tea, Tambe Milind, Gams Matjaž. A 1. probabilistic risk analysis for multimodal entry control. Expert Systems with Applications, 2011, 38 (6), 6696-6704.
- Scheubert Lena, Schmidt Rainer, Repsilber Dirk, Luštrek Mitja, Fuellen 2. Georg. Learning biomarkers of pluripotent stem cells in a mouse. DNA Research, 2011, 18 (4), 233-251.
- 3. Pogorelc Bogdan, Bosnić Zoran, Gams Matjaž. Automatic recognition of gait-related health problems in the elderly using machine learning. Multimedia Tools and Applications, 2011, 1-22.
- Piltaver Rok, Luštrek Mitja, Gams Matjaž. The pathology of heuristic Technology we received the Taras Award for a successful collaboration 4. search in the 8-puzzle. Journal of Experimental and Theoretical Artificial between a research institution and industry. It was awarded to the iLab Intelligence, 2011.
- 5. Vidulin Vedrana, Gams Matjaž. Impact of high-level knowledge on economic welfare through interactive data mining. Applied Artificial Intelligence, 2011, 25 (4), 267–291.
- 6. Dovgan Erik, Luštrek Mitja, Pogorelc Bogdan, Gradišek Anton, Burger Helena, Gams Matjaž. Intelligent elderly-care prototype for fall and disease detection = Inteligentni prototip za oskrbo starejših, ki zaznava padce in bolezni. Slovenian Medical Journal, 2011, 80 (11), 824-831.

project.

## Patent application

1 Erik Dovgan, Matjaž Gams, Rok Piltaver, Gašper Pintarič, Andrej Planina, Bogdan Pogorelc: Intelligent surveillance system and procedure for detection of unusual behaviour, patent pending, application nr. 201100298, Ljubljana, 5. 8. 2011

We received the Taras Award for a successful collaboration between a research institution and industry, and the Silver Award at the Slovenian Innovation Forum for the Pedius system for the computer-supported restoration of wall paintings.

## Awards and appointments

- Erik Dovgan: Best graduate student paper award at the Genetic and Evolutionary Computation (GECCO 2011) 1. Conference, "A multiobjective optimization algorithm for discovering driving strategies", Dublin, Ireland, 12.-16.7.2011
- 2. Bogdan Filipič, Miha Mlakar, Erik Dovgan, Tea Tušar: Silver award for excellence of innovative industries at the 6th Slovenian Innovation Forum for Pedius, a system for computer-aided reconstruction of wall paintings, Ljubljana, 23. 11. 2011
- Boštjan Kaluža: Best ICT paper award at the 3rd Jožef Stefan International Postgradu-3. ate School Students Conference for the paper "Identifying suspicious behaviour from multiple events", Ljubljana, 25. 5. 2011
- 4. Tomaž Kompara: Dean's praise for the best students in academic year 2010/2011, University of Ljubljana, Faculty of Electrical Engineering, Ljubljana, 29. 11. 2011
- Damjan Kužnar, Matjaž Gams, Blaž Mahnič, Domen Marinčič, Rok Piltaver: TARAS 5. award at the 3rd Industrial Forum of Innovation, Portorož, R&D and Technology (IRT) for successful collaboration between research institution and industry, project "Intelligent Laboratory System for Healthcare (iLab)", 6. 6. 2011

## Organization of conferences, congress and meetings

- 1. 3rd Jožef Stefan International Postgraduate School Students Conference, Jožef Stefan Institute, Ljubljana, 25. 5. 2011
- 4th International Workshop on Semantic Ambient Media Experiences, in conjunction 2. with C&T 2011, Brisbane, Australia, 29. 6.-2. 7. 2011
- 18th Workshop on Nature-Inspired Algorithms, AVN, Jožef Stefan Institute, Ljubljana, 3. 13.9.2011



Figure 5: Little Dragon - a virtual assistant answering questions about the Municipality of Ljubljana



- 4. 14th International Multiconference Information Society, IS 2011, 10.–14. 10. 2011 independent conferences:
  Intelligent Systems,
  - Facing Demographic Challenges,
  - Cognitive Sciences,
  - Collaboration, Software and Services in Information Society,
  - Data Mining and Data Warehouses,
  - Education in Information Society,
  - Cognitronics,
  - Robotics,
  - Internet and Slovenia: 1985-1995

## INTERNATIONAL PROJECTS

- 1. Robots Bootstrapped through Learning from Experience Xperience
  - 7. FP, 270273
  - EC; Karlsruhe Institute of Technology, Karlsruhe, Germany
- Prof. Matjaž Gams, Asst. Prof. Aleš Ude
  Micro-Request-Based Aggregation, Forecasting and Scheduling of Energy Demand, Supply and Distribution
  - MIRACLE, MIRABEL
  - 7. FP. 248195
  - EC; Sofía Martínez-Schmitt, Dr. Henrike Berthold, SAP AG, Walldorf, Germany Prof. Bogdan Filipič
- 3. Ubiquitous Care System to Support Independent Living CONFIDENCE
- 7. FP, 214986

EC; Centro de Estudios e Investigaciones Tecnicas de Guipuzcoa, San Sebastian, Spain Prof. Matjaž Gams, Prof. Leon Žlajpah

- 4. European Urban Simulation for Asymmetric Scenarios EUSAS Contract EADS DC
- EADS N.V., Defense and Security Systems, Elancourt, France Prof. Matjaž Gams
- Cyclic and Person-Centric Health Management: Integrated Approach for Home, Mobile and Clinical Environments
  - CHIRON, ARTEMIS FIMI S.R.L, Italy
  - Dr. Mitja Luštrek
- 6. Constrained Multiobjective Optimization Based on Simulation Models BI-FI/11-12-018
  - Dr. Erkki Laitinen, University of Oulu, Faculty of Science, Department of Mathematical

## MENTORING

### M. Sc. Theses

- 1. Hristijan Gjoreski, Adaptive human activity recognition and fall detection using wearable sensors (mentor Matjaž Gams).
- Vidojka Srebrnič, Optimization of vegetable food supply using linear programming (mentor Bogdan Filipič).

## VISITORS FROM ABROAD

- 1. dr. Holger Bracker, Cassidian, Unterschleissheim, Germany, 27.-28. 1. 2011
- Mark Contat, Cassidian SAS, Val-de-Reuil Cedex, France, 27.–28. 1. 2011
- Štefan Dlugolinský, Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia, 27.–28. 1. 2011
- 4. Łukasz Dutka, ACK Cyfronet AGH, Kraków, Poland, 27.-28. 1. 2011
- Ladislav Hluchý, Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia, 27.–28. 1. 2011
- 6. mag. Bartosz Kryza, ACK Cyfronet AGH, Kraków, Poland, 27.-28. 1. 2011
- Marcel Kvassay, Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia, 27.–28. 1. 2011
- dr. Michal Laclavik, Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia, 27.–28. 1. 2011
- 9. Mikael Lundin, Swedish Defence Research Agency FOI, Stockholm, Sweden, 27.-28. 1. 2011
- 10. dr. Bernhard Schneider, Cassidian, Unterschleissheim, Germany, 27.–28. 1. 2011
- dr. Martin Šeleng, Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia, 27.–28. 1. 2011

Sciences, Oulu, Finland Prof. Bogdan Filipič

## 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

## RESEARCH PROGRAM

1. Artificial Intelligence and Intelligent Systems Prof. Matjaž Gams

## NEW CONTRACT

- Cooperation in the introduction, use and financing of the "Intelligent doors and windows" project Intech - Les, d. o. o.
  - Prof. Matjaž Gams
- 12. Michał Wrzeszcz, ACK Cyfronet AGH, Kraków, Poland, 27.-28. 1. 2011
- prof. dr. Vladimir A. Kulyukin, Department of Computer Science Utah State University Logan, Utah, United States, 20.–23. 5. 2011
- prof. dr. Norbert Kroo, Hungarian Academy of Science, Budapest, Hungary, 11. 10. 2011
   dr. Zoran Stančič, Information Society and Media Directorate-General, European Commision, Brussels, Belgium, 11. 10. 2011
- 6. prof. dr. Angelo Montanari, Department of Mathematics and Computer Science, University of Udine, Udine, Italy, 12.–14. 10. 2011
- prof. dr. Christopher W. Geib, School of Informatics, University of Edinburgh, Edinburgh, United Kingdom, 14. 10. 2011
- dr. Roberta Gazzarata, Department of Computer and System Sciences, University of Genoa, Genoa, Italy, 6.–9. 11. 2011
- prof. dr. Mauro Giacomini, Faculty of Engineering, University of Genoa, Genoa, Italy, 6.–9. 11. 2011
- 20. Philip Needham, Cardionetics, LTD., Fleet Hampshire, United Kingdom, 6.-10. 11. 2011
- 21. Luigi Albani, FIMI S.r.l., Saronno, Italy, 7.-10. 11. 2011
- prof. dr. Boldizsar Bencsath, Department of Telecommunications, Budapest University of Technology and Economics, Budapest, Hungary, 7.–9. 11. 2011
- dr. Luca Becchetti, Department of Computer and System Sciences Antonio Ruberti, Sapienza University of Rome, Rome, Italy, 7.–10. 11. 2011
- 24. Silvio Bonfiglio, FIMI S.r.l., Saronno, Italy, 7.-10. 11. 2011
- prof. dr. Levente Buttyan, Department of Telecommunications, Budapest University of Technology and Economics, Budapest, Hungary, 7.–9. 11. 2011
- Angelo Capossele, Department of Computer Science, Sapienza University of Rome, Rome, Italy, 7.–9. 11. 2011
- 27. Petros Chondros, Industrial Systems Institute (ISI), Athens, Greece, 7.-10. 11. 2011
- 28. Letizia Gabbrielli, Elsag Datamat, Genoa, Italy, 7.-10. 11. 2011
- 29. John Gialelis, Industrial Systems Institute (ISI), Athens, Greece, 7.-10. 11. 2011
- 30. dr. Miguel A. González Ballester, Alma IT Systems, Barcelona, Spain, 7.-9. 11. 2011
- dr. Gabriele Guarnieri, Department of Industrial Engineering and Information Technology, University of Trieste, Trieste, Italy, 7.–9. 11. 2011

- 32. Maitena Ilardia, ESI-Tecnalia, Bilbao, Spain, 7.-9. 11. 2011
- 33. dr. Artur Krukowski, Intracom Telecom S. A., Athens, Greece, 7.-9. 11. 2011
- 34. prof. dr. Claudio Lamberti, Department of Electronics, Computer Science and Systems, University of Bologna, Bologna, Italy, 7.-9. 11. 2011
- 35. dr. Nico Lanconelli, Department of Physics, University of Bologna, Bologna, Italy, 7.-9.11.2011
- 36. dr. Michele Magno, Department of Electronics, Computer Science and Systems, University of Bologna, Bologna, Italy, 7.-9. 11. 2011
- 37. dr. Cédric Marchessoux, Barco, Kortrijk, Belgium, 7.-10. 11. 2011
- 38. prof. dr. Gaia Maselli, Department of Computer Science, Sapienza University of Rome, Rome, Italy, 7.-9. 11. 2011
- 39. Evangelos B. Mazomenos, School of Electronics and Computer Science, University of Southampton, Southampton, United Kingdom, 7.-10. 11. 2011
- 40. prof. dr. Francesco Morandi, Faculty of Economics, University of Sassari, Sassari, Italy, -9.11.2011
- 41. Gianni Pizzetti, Elsag Datamat, Genoa, Italy, 7.-10. 11. 2011
- 42. prof. Giovanni Ramponi, Department of Industrial Engineering and Information Technology, University of Trieste, Trieste, Italy, 7.-9. 11. 2011

- 43. Juan Maria Rodriguez Anta, Atos International, Madrid, Spain, 7.-10, 11, 2011
- 44. Laura Lara Rodríguez, Alma IT Systems, Barcelona, Spain, 7.-9. 11. 2011
- 45. Alberto Rugnone, Healthcare & Telecare Team Technical Lead, I+, Bologna, Italy, 7.-9.11.2011
- 46. mag. Aurora Summa, INAIL Prosthesis Centre, Bologna, Italy, 7.-9. 11. 2011
- prof. dr. Fabio Vergari, Faculty of Mechanical Engineering, University of Bologna, Bologna, Italy, 7.–9. 11. 2011 47.
- 48. Jan-Marc Verlinden, ZorgGemak BV, AK Leiden, Netherlands, 7.-10. 11. 2011 49. Paolo Emilio Puddu, Department of Cardiovascular Pathophysiology, Anaesthesiology
- and Surgery, Sapienza University of Rome, Rome, Italy, 8.-10. 11. 2011
- 50. dr. Héctor Solar, CEIT, San Sebastián, Spain, 8.-10. 11. 2011
- 51. Luca Filipponi, WLAB srl, Rome, Italy, 9.-10. 11. 2011
- 52. Gennaro Tartarisco, Institute of Clinical Phisiology CNR, Pisa, Italy, 9. 11. 2011
- 53. dr. Dalkhat Ediev, Vienna Institute of Demography, Austrian Academy of Sciences, Vienna, Austria, 10.-11. 10. 2011
- 54. prof. dr. Vladimir A. Fomichov, Higher School of Economics, Faculty of Business Informatics, Moscow, Russia, 10.–11. 11. 2011

## STAFF

#### Researchers

- Prof. Ivan Bratko\* 1.
- Asst. Prof. Aleš Dobnikar\* 2.
- Prof. Bogdan Filipič 3.
- 4. Prof. Matjaž Gams, Head
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- Prof. Vladislav Rajkovič\*\*\* 6.
- Dr. Tomaž Šef

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- 10. Dr. Matej Guid\* 11. Dr. Domen Marinčič
- 12. Dr. Aleksander Pivk\*

#### Postgraduates

- 13. Andrej Bratko\*, B. 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.
- 19. Jana Krivec\*, B. Sc.
- 20. Damjan Kužnar, B. Sc.
- 21. Miha Mlakar, B. Sc.

## BIBLIOGRAPHY

## ORIGINAL ARTICLES

- 1. Robert Blatnik, Gorazd Kandus, Tomaž Šef, "Influence of the perceptual speech quality on the performance of the text-independent speaker recognition system", Int. j. circuits syst. signal process., vol. 5, no. 4, pp. 346-353, 2011.
- 2. Ivan Bratko, "Autonomous discovery of abstract concepts by a robot", In: Adaptive and natural computing algorithms: 10th international conference, ICANNGA 2011, Ljubljana, Slovenia: proceedings, Lect. notes comput. sci., vol. 6593, pp. 1-11, 2011.
- 3. Erik Dovgan, Mitja Luštrek, Bogdan Pogorelc, Anton Gradišek, Helena Burger, Matjaž Gams, "Intelligent elderly-care prototype for fall and disease detection", Zdrav Vestn (Tisk. izd.), vol. 80, no. 11, pp. 824-831, 2011.
- 4. Vida Groznik, Matej Guid, Aleksander Sadikov, Martin Možina, Dejan Georgiev, Veronika Kragelj, Samo Ribarič, Zvezdan Pirtošek, Ivan Bratko, "Elicitation of neurological knowledge with ABML", In: Artificial intelligence in medicine: proceedings, Lect. notes comput. sci., vol. 6747, pp. 14-23, 2011.
- 5. Matej Guid, Ivan Bratko, "Using heuristic-search based engines for estimating human skill at chess", ICGA journal, vol. 34, no. 2, pp. 71-81, 2011.

- 6. Boštjan Kaluža, Erik Dovgan, Tea Tušar, Milind Tambe, Matjaž Gams, "A probabilistic risk analysis for multimodal entry control", Expert syst. appl., vol. 38, no. 6, pp. 6696-6704, 2011.
- Aljaž Košmerlj, Ivan Bratko, Jure Žabkar, "Embodied concept discovery through qualitative action models", Int. j. uncertain. fuzziness knowl.*based syst.*, vol. 19, no. 3, pp. 453-475, 2011. 8. Andrej Oblak, Ivan Bratko, "Learning from noisy data using a non-
- covering ILP algorithm", In: Inductive logic programming: 20th International Conference, ILP 2010, Florence, Italy: revised papers, Lect. notes comput. sci., vol. 6489, pp. 190-197, 2011.
- 9. Dejan Petelin, Bogdan Filipič, Juš Kocijan, "Optimization of Gaussian process models with evolutionary algorithms", In: Adaptive and natural computing algorithms: 10th international conference, ICANNGA 2011, Ljubljana, Slovenia: proceedings, Lect. notes comput. *sci.,* vol. 6593, pp. 420-429, 2011.
- 10. Rok Piltaver, Erik Dovgan, Matjaž Gams, "An intelligent indoor surveillance system", Informatica (Ljublj.), vol. 35, no. 3, pp. 383-390, 2011.
- 11. Bogdan Pogorelc, Zoran Bosnić, Matjaž Gams, "Automatic recognition of gait-related health problems in the elderly using machine learning", Multimedia tools and applications, pp. [1-22], 2011.

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25. Bogdan Pogorelc\*, B. Sc.

28. Vedrana Vidulin, B. Sc.

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- 46. Tea Tušar, Erik Dovgan, Bogdan Filipič, "Scheduling of flexible electricity production and consumption in a future energy data management system: problem formulation", In: *Zbornik 14. mednarodne multikonference Informacijska družba - IS 2011, 10-14. oktober 2011: zvezek A: volume A,* (Informacijska družba), Marko Bohanec, ed., Matjaž Gams, ed., Dunja Mladenić, ed., Marko Grobelnik, ed., Marjan Heričko, ed., Urban Kordeš, ed., Olga Markič, ed., Jadran Lenarčič, ed., Leon Žlajpah, ed., Andrej Gams, ed., Vladimir Fomichov, ed., Olga S. Fomichova, ed., Andrej Brodnik, ed., Rok Sosič, ed., Vladislav Rajkovič, ed., Tanja Urbančič, ed., Mojca Bernik, ed., Ljubljana, Institut Jožef Stefan, 2011, pp. 96-99.
- 47. Tea Tušar, Bogdan Filipič, "Visualizing 4D approximation sets of multiobjective optimizers with prosections", In: *GECCO'11 proceedings and companion*, 13th Annual Genetic and Evolutionary Computation Conference, July 12-16, 2011, Dublin, Ireland, New York, ACM, = Association for Computing Machinery, cop. 2011, pp. 737-744.

## B. Sc. Thesis

1. Tomaž Kompara, *Automatic question classification according to the answer type:* undergraduate thesis, Ljubljana, [T. Kompara], 2011.

## PATENT APPLICATION

1. Matjaž Gams, Rok Piltaver, Erik Dovgan, Andrej Planina, Gašper Pintarič, Bogdan Pogorelc, *Intelligent surveillance system and procedure for detection of unusual behaviour*, P-201100298, Urad RS za intelektualno lastnino, 5.8.2011.

## 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. The topics include modelling basic thermal hydrodynamic phenomena, thermal-hydraulic safety analyses of design-basis and severe accidents, structural safety analyses and probabilistic safety assessment. Most research activities are part of international cooperation programmes. Research results are incorporated into the projects for the industry and for the regulatory authorities, as well as in the under-graduate and doctoral-studies programmes.

#### Modelling of basic thermal hydrodynamic phenomena

Within the research of convective boiling, we continued the simulations of boiling flow experiments in a vertical rectangular channel, performed at the Texas A&M University (USA). The simulations were performed with the NEPTUNE\_CFD computer code. We introduced a method for the evaluation of modelling uncertainty, in which we systematically assessed the uncertainty of the bubble departure model that is one of the key parameters of the boiling flow process. The work was performed within the NURISP project co-financed by the European Commission within the 7<sup>th</sup> framework programme (EC, 7<sup>th</sup> FP).

The modelling of turbulent flow is being used in the research related to the development of future fission and fusion reactor systems. We performed direct numerical simulations of the turbulent heat transfer in the channels at Prandtl number 0.01. These simulations took into account the heat conduction in the fuel and resulted in a detailed analysis of the temperature fluctuations inside the fuel that are induced by the turbulent flow. Research

was carried out within the project THINS (EC, 7th FP) and is relevant for the next-generation nuclear fission reactors that will be cooled with liquid sodium. In the frame of the development of the DEMO fusion reactor concept, we have studied the divertor performance cooled by helium jets. Using computer simulations, we have analyzed the influence of two different arrangements of nozzles on the efficiency of the cooling of a hot plate.

Calculated distributions of the Nusselt numbers were compared with the experimental results. These activities were carried out in collaboration with the Karlsruhe Institute of Technology (Germany) within the European Fusion Development Association (EFDA).

Various transients in a single- or two-phase (gas-liquid) flow may occur in the piping systems of nuclear plants during design-basis accidents. In the field of transient modelling, the one-dimensional WAHA computer code has been further developed. New models of the two-phase stratified and slug flow were tested with the simulations of a condensation-induced water hammer in a horizontal pipe. This activity was part of the NURISP project. The WAHA code is also being tested at supercritical temperatures and pressures, at which some of the next-generation nuclear reactors, cooled with supercritical water, are designed to operate. These studies were performed within a bilateral cooperation with KFKI (Hungary).

A steam explosion might occur during a hypothetical severe accident in a nuclear power plant if the molten reactor core were to pour into the water in the reactor cavity. Within the OECD project SERENA, we simulated and analyzed, using the European code MC3D, the steam explosion experiments that were performed on the complementary KROTOS (Commissariat à l' Energie Atomique - CEA, France) and TROI (Korea Atomic Energy Research Institute) facilities. We performed a comprehensive steam-explosion analysis in a typical boiling-water reactor and in a typical pressurized-water reactor for various scenarios of the release of the molten reactor core. We analyzed the influence of the jet-breakup modelling and the melt-droplet solidification modelling on the fuel-coolant interaction and the steam explosion strength. These activities are being carried out within the SARNET-2 network of excel- Figure 1: Simulation of a steam explosion in a typical pressurized water lence (EC, 7th FP) as well.

The modelling of turbulent flow is being used in the research for the development of future fission and fusion reactor systems.



MELEAF

Prof. Leon Cizelj

Head



reactor with the European fuel-coolant interaction code MC3D.

#### Thermal-hydraulic safety analyses

The TRAC/RELAP Advanced Computational Engine (TRACE) is the latest in a series of advanced, best-estimate reactor-system computer codes developed by the U.S. Nuclear Regulatory Commission. At the JSI, the TRACE code

The TRACE thermal-hydraulic computer code was used for the first time at the JSI to simulate the experiments in the ACHILLES and BETHSY facilities. was applied for the first time to simulate experiments, performed in the ACHILLES (United Kingdom Atomic Energy Authority) and BETHSY (CEA) facilities. The input decks of these facilities, which were already developed for the RELAP5 code within the participation in the OECD International Standard Problems Nos. 25 and 27, were converted for the TRACE code. In general, the results of the simulations with the TRACE code show a good agreement

with the experimental data for the natural reflood test in the ACHILLES facility, and the BETHSY 9.1b and 6.2TC tests (2-inch and 6-inch cold leg break without a high-pressure safety injection).

In the field of modelling containment phenomena, we have simulated, using the Computational Fluid Dynamics code CFX, an experiment of an air-helium atmosphere-stratification breakup, using the natural circulation caused by heating the containment wall. The experiment was performed in the MISTRA experimental facility (CEA) within the OECD SETH-2 project. We continued simulations of the hydrogen-combustion experiments performed in the ENACCEF facility in the ICARE centre at the Centre National de la Recherche Scientifique in Orléans (France), using the CFX code and the lumped-parameter CONTAIN code. We also simulated the natural circulation during an experiment in the TOSQAN experimental facility (Institut de Radioprotection et de Sûreté Nucléaire, France) using the European severe-accident code ASTEC and the CONTAIN code.

#### Structural safety analyses

Recent research has been focused towards the development of the 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 the experimental (e.g., X-ray diffraction



Figure 2: Simulation of a loop seal clearing in the BETHSY experimental facility (CEA, Grenoble, France).

contrast tomography) or analytical (e.g., Voronoi tessellation) methods. The loading of the randomly shaped and oriented crystal grains with anisotropic properties results in highly nonhomogeneous microscopic stress fields, which are estimated by using the finite element solver ABAQUS.

In 2011 the first method for simulating the initiation and growth of intergranular cracks has been developed. The grain boundaries are modelled explicitly from the measured data on the shapes and orientation of the grains within a stainless steel wire. The measurements were performed using the diffraction contrast tomography by the University of Manchester (UK). The relative susceptibility of a particular grain boundary in the model depends mainly on the orientation of the neighbouring grains. The first results confirm the feasibility of the method and they support further developments, especially towards the calibration of the material parameters. The development of the simulation method benefits from the collaboration with the Joint Research Center (JRC) of the European Commission in Petten (The Netherlands).

Also in 2011, two new research projects were developed in cooperation with our partners to be launched in early 2012. The first is devoted to the initiation and propagation of the cracks in dissimilar welds between austenitic and ferritic steels. The project named MULTIMETAL will be co-financed

by the European Commission as a part of the 7<sup>th</sup> FP. The second project aims at predicting the fatigue of the piping containing intensive turbulent mixing of fluids with different temperatures. This project was developed by the members of the European network of excellence on the nuclear plant-lifetime prediction NULIFE (EC,  $6^{th}$  FP) that, in 2011, successfully completed a transition towards the non-profit professional association NUGENIA.

#### Probabilistic safety assessment

An analysis of the station-blackout initiating event and repercussions on the safety of the nuclear power plant (NPP), in light of the accident in the Fukushima Daiichi NPP (Japan) following the Great East Japan Earthquake of March 11, 2011, was performed. The implications of the extension of the station-blackout coping capability on the safety of the NPP was analyzed with the state-of-the-art probabilistic and deterministic methods applied on the reference models of the NPPs. The obtained results show a large decrease in the core-damage frequency with an extension of the station-blackout coping capability.

An analysis of the modification of the NPP parameters resulting from the subsynchronous-resonance phenomenon has been performed. The obtained results showed that the subsynchronous resonance results in a short and fast transient. A large change of the primary coolant-system parameters was

observed in the calculated results. A new method for the reliability and vulnerability analysis of an electrical power system was developed. The method, which considers the operational parameters of the analyzed power system, was applied on the reference power system representing the Swiss system. The most important interconnections

A new method for reliability and vulnerability analyses of an electrical power system was developed.

and substations were identified in the obtained results. The work was performed in cooperation with Eidgenössische Technische Hochschule Zürich.

A method for optimization of the testing and the maintenance of the stand-by safety systems in a nuclear plant has been developed, which was supported by the development of our own computer code. The genetic algorithms are integrated into the method, which enables a multi-objective optimization of the related parameters.

#### Technical cooperation, consulting services and education

In 2011 the Reactor Engineering Department researchers also cooperated in the projects for the industry. As an authorized institution for the radiation and nuclear safety, we performed a verification of the Krško NPP station-

blackout-analysis results with a special emphasis on the containment and the spent-fuel pit response. The Krško NPP provided this analysis in response to the Western European Nuclear Regulators' Association (WENRA) requirements for "stress tests" after the accident in the Fukushima Daiichi NPP. In the framework of the regular Krško NPP activities relating to the maintenance and the improvements of nuclear safety, two projects are currently in pro-

### We contributed to the information for the general public on the developments in the Fukushima Daiichi Nuclear Power Plant.

gress: a safety assessment of the  $3^{rd}$  emergency diesel-generator implementation and an evaluation of the safety analysis for the  $2^{rd}$  periodic safety analysis.

The members of the department are also actively involved in the nuclear engineering under-graduate and doctoral-studies programmes 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.

The results of our long-term research activities in the field of nuclear safety have also facilitated more than 50 contributions of the departmental members towards informing the general public about the developments in the Fukushima Daiichi Nuclear Power Plant.

## Some outstanding publications in the last year

- 1. B. Končar, I. Simonovski, M. Draksler, Influence of multiple jet cooling on the heat transfer and thermal stresses in DEMO divertor cooling finger, *Fusion Engineering and Design*, vol. 25, pp. 537-548, 2011.
- I. Simonovski, L. Cizelj, Computational multiscale modeling of intergranular cracking, *Journal of Nuclear Materials*, vol. 414, pp. 243-250, 2011.
- 3. D. Kančev, B. Gjorgiev, M. Čepin, Optimization of test interval for ageing equipment: a multi-objective genetic algorithm approach, *Journal of Loss Prevention in the Process Industries*, vol. 24, pp. 397-404, 2011.

## Awards and appointments

- 1. Adrien Giacosa: Best Poster Award, Bovec, Nuclear Society of Slovenia, Analysis and Sensitivity Study of BWR Ex-Vessel Steam Explosion with MC3D Code, co-authored by Mitja Uršič and Matjaž Leskovar
- 2. Samo Košmrlj: Young Authors Award, Bovec, Nuclear Society of Slovenia, Transient Analysis of the Divertor Cooling Finger Subjected to High Cyclic Surface Heating, co-authored by Boštjan Končar
- 3. Andrej Prošek: Founding member recognition for the contribution in the establishment of the Nuclear Society of Slovenia, Ljubljana, Nuclear Society of Slovenia
- 4. Mitja Uršič: ENEN Prize, Nice, France, ENEN, Modeling of solidification effect in fuel-coolant interactions

## Organization of conferences, congress and meetings

- 1. SNE TP Governing Board Meeting, Grand Hotel Union, Ljubljana, 5 October 2011
- 2. SARNET Management Team Meeting, Jožef Stefan Institute, Ljubljana, 27 October 2011

## INTERNATIONAL PROJECTS

- 1. New MS Linking for an Advanced Cohesion in Euratom Research NEWLANCER 7. FP. 295826 EC; Daniela Diaconu, Institute for Nuclear Research - Pitesti, Arges, Romania Prof. Leon Cizeli 2. Training Scheme on Nuclear Safety Culture TRASNUSAFE 7. FP - EURATOM, 249674 EC; Giuseppe Esposito, Universite Catholique de Louvain, Louvain-la-Neuve, Belgium Prof. Borut Mavko 3. Thermal-hydraulics of Innovative Nuclear Systems THINS 7. FP - EURATOM, 249337 EC; Dr. Xu Cheng, Karlsruher Institut für Technologie (KIT), Institute for Neutron Physics and Reactor Technology, Eggenstein-Leopoldshafen, Germany Prof. Iztok Tiseli European Nuclear Education Network Training Schemes 4. ENEN-III 7. FP - EURATOM, 232629 EC; Dr. Peter De Regge, ENEN Association, European Nuclear Education Network Association p/a Centre CEA de Saclay, Gif-sur-Yvette, France Prof. Leon Cizeli 5. Network of Excellence for a Sustainable Integration of European Research on Severe Accident Phenomenology and Management - Phase 2 SARNET 2 7. FP - EURATOM, 231747 EC; IRSN, Fontenay-aux-Roses, France Dr. Matiaž Leskovar Nuclear Reactor Integrated Simulation Project 6. NURISP 7. FP - EURATOM, 232124 EC; Commissariat a l'Energie Atomique (CEA), Paris, France Prof. Iztok Tiselj Divertor High Flux Helium Cooling - 4.5.1. FU 7 7. FP - EURATOM, Slovenian Fusion Association – SFA 3211-08-000102, FU07-CT-2007-00065 EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Dr. Boštjan Končar 8 Nuclear Plant Life Prediction NULIFE 6. FP, 036412 EC; Valton Teknillinen Tutkimuskeskus (VTT), Espoo, VTT, Finland Prof. Leon Cizelj
- Steam Explosion Resolution for Nuclear Applications SERENA

OECD/NEA

Jean Gauvain, OECD Nuclear Energy Agency, Agence de l'OECD pour l'Energie Nucleaire, Issy-les-Moulineaux, France Dr. Matjaž Leskovar

 Code Applications and Maintenance Program (CAMP) Thermal-Hydraulic Code Applications and Maintenance International Research Project

Dr. Andrew J. Szukiewicz, Reactor and Plant Systems Branch, Division of Systems Technology, Office of Nuclear Regulatory Research;

Dr. Ashok C. Thadani, Director, Donna-Maria Perez, Office of Nuclear Regulatory

Research, United States Nuclear Regulatory Commission (US NRC), Washington, D. C., USA Part Marike

Prof. Borut Mavko

## MENTORING

## Ph. D. Thesis

1. Mitja Uršič, Modelling of solidification effects in fuel-coolant interactions (mentor Borut Mavko; co-mentor Matjaž Leskovar).

#### M. Sc. Theses

- Raphaël Connes, Scaling of simulation of hydrogen combustion with ASTEC computer code from containment experimental facility to actual containment (mentor Ivo Kljenak).
- Adrien Giacosa, Steam explosions analysis in reactor conditions (mentor Matjaž Leskovar).

 Fluid-fluid Transition and Related Phenomena in Flowing Systems 601
 Dr. Imre Attila, MTA KEKI Atomic Energy Research Institute, Budapest

Dr. Imre Attila, MTA KFKI Atomic Energy Research Institute, Budapest, Hungary Prof. Iztok Tiselj

- 12. Simulation of hydrogen combustion experiments in the ENACCEF experimental facility Commissariat a l'Energie Atomique (CEA), Paris, France Asst. Prof. Ivo Kljenak
- Modelling of condensation induced water hammer and boiling crisis in subcooled boiling flow Commissariat a l'Energie Atomique (CEA), Grenoble, France
- Dr. Boštjan Končar
- 14. Analyses of ex-vessel molten fuel coolant interaction CEA Cadarache, Commisariat á l'é atomique et aux énergies alternatives, Saint Paul lez Durance, France Dr. Matjaž Leskovar
- Application and validation of multiscale method for two-phase flow analyses in nuclear reactors
- Commissariat a l'Energie Atomique (CEA), Grenoble, France Dr. Boštjan Končar
- 16. Simulations of atmosphere stratification breakup experiments with lumped-parameter codes

Commissariat a l'Energie Atomique (CEA), Saclay, France Asst. Prof. Ivo Kljenak

## R & D GRANTS AND CONTRACTS

- 1. Direct contact condensation in stratified two-phase flow Prof. Iztok Tiselj
- 2. 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 Mavko
- Development of methods and models for simulation of thermal-hydraulic phenomena in innovative nuclear reactors Prof. Iztok Tiselj

## RESEARCH PROGRAM

1. Nuclear Engineering Prof. Borut Mavko

## NEW CONTRACT

 Project "Severe Accident Management" Gen d. o. o. Dr. Matjaž Leskovar

## VISITORS FROM ABROAD

- Mr. Alexandre Vigouroux, B. Sc., Institute Catholique d'Arts et Métiers (ICAM), Nantes, France, 6 July 2010 to 31 January 2011
   Mr. Dinesh Singh, B. Sc., Indian Institute of Technology (IIT) Bombay, Mumbay, India,
- 2. Mr. Dinesh Singh, B. Sc., Indian Institute of Technology (IIT) Bombay, Mumbay, India, 6 December 2010 to 10 January 2011
- Mr. Adrien Giacosa, B. Sc., National Institute of Nuclear Science and Technology (INSTN), Saclay, France, 1 April to 31 December 2011
- Mr. Raphaël Connes, B. Sc., National Institute of Nuclear Science and Technology (INSTN), Saclay, France, 1 April to 31 August 2011
- Mrs. Alexandra Sitdikova, B. Sc., Tomsk Polytechnic University (TPU), Tomsk, Rusia, 13 July to 1 November 2011
- Dr. Imre Barna, Atomic Energy Research Institute (AEKI), Budapest, Hungary, 25 to 27 October 2011

- Dr. Attila Imre, Atomic Energy Research Institute (AEKI), Budapest, Hungary, 25 to 27 7. October 2011
- 8 Mr. Gaurang Sharma, B. Sc., Indian Institute of Technology (IIT) Bombay, Mumbay, India, 12 December 2011 to 6 January 2012

Student visitors within the International Association for the Exchage of Students for Technical Experience (IAESTE):

- Mr. David McCourt, B. Sc., Swinburne University of Technology, Hawthorn, Australia, 1 1. August to 24 October 2011
- 2 Mr. Graham Alasdair Bruce, B. Sc., Durham University, Durham City, United Kingdom, 15 August to 23 September 2011

## **STAFF**

#### Researchers

- 1. Prof. Leon Cizelj, Head
- Prof. Marko Tomaž Čepin\*
- Ljubo Fabjan, M. Sc. 3.
- 4. Asst. Prof. Ivo Kljenak
- Dr. Boštjan Končar 5.
- Dr. Matjaž Leskovar 6.
- Asst. Prof. Marko Matkovič 7. 8. Prof. Borut Mavko
- Dr. Andrej Prošek
- 10.
- Prof. Iztok Tiselj 11. Dr. Andrija Volkanovski

#### Postdoctorial associates

- 12. Dr. Samir El Shawish
- 13. Dr. Mihaela Irina Uplaznik
- 14. Dr. Mitja Uršič
- Postgraduates

15. Ovidiu-Adrian Berar, B. Sc.

## BIBLIOGRAPHY

## **ORIGINAL ARTICLES**

- 1. Alberto Cavallini, Stefano Bortolin, Davide Del Col, Marko Matkovič, Luisa Rossetto, "Condensation heat transfer and pressure losses of high- and low-pressure refrigerants flowing in a single circular minichannel", *Heat transf. eng.*, vol. 32, no. 2, pp. 90-98, 2011.
- 2. Alberto Cavallini, Davide Del Col, Marko Matkovič, Luisa Rossetto, "Pressure drop during two-phase flow of R134a and R32 in a single minichannel", J. heat transfer, vol. 131, no. 3, pp. 033107-1-033107-8, 2011.
- 3. Leon Cizelj, "Jedrska energija danes in jutri: pomemben globalni vir električne energije", Geogr. šoli, vol. 20, no. 2, pp. 24-31, 2011.
- 4. Leon Cizelj, Igor Simonovski, "Fatigue relevance of stratified flows in pipes: a parametric study", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1191-1195, 2011. 5. Marko Čepin, "Risk-informed decision-making related to the on-line
- maintenance", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1114-1118, 2011.
- 6. Davide Del Col, Stefano Bortolin, Alberto Cavallini, Marko Matkovič, "Effect of cross sectional shape during condensation in a single square minichannel", Int. j. heat mass transfer, vol. 54, no. 17/18, pp. 3909-3920, 2011.
- 7. Martin Draksler, Boštjan Končar, "Analysis of heat transfer and flow characteristics in turbulent impinging jet", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1248-1254, 2011.
- 8. Samir El Shawish, Jure Dobnikar, Emmanuel Trizac, "Colloidal ionic complexes on periodic substrates: ground-state configurations and pattern switching", Phys. rev., E Stat. nonlinear soft matter phys. (Print), vol. 83, no. 4, pp. 041403-1-041403-10, 2011.
- 9. Duško Kančev, Marko Čepin, "Evaluation of risk and cost using an agedependent unavailability modelling of test and maintenance for stand by components", J. loss prev. process ind., vol. 24, no. 2, pp. 146-155, 2011.
- 10. Duško Kančev, Marko Čepin, "The price of risk reduction: optimization of test and maintenance integrating risk and cost", In: Special issue on

- 16. Raphael Stephane Connes, B. Sc.
- 17. Oriol Costa Garrido, B. Sc.
- 18. Martin Draksler, B. Sc
- 19. Blazhe Gjorgiev, B. Sc.
- 20. Romain Claude Francis Henry, B. Sc.
- 21. Duško Kančev, B. Sc.
- 22. Blaž Mikuž, B. Sc.
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- 24. Andrej Sušnik, B. Sc.

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- 25. Tanja Klopčič
- 26. Zoran Petrič, B. Sc.
- 27. Nataša Pouh, B. Sc. 28. Zlata Vrhovec Mikolič, retired 04.07.11

Note: \* part-time JSI member

> the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1119-1125, 2011.

- 11. Duško Kančev, Blaže Gjorgiev, Marko Čepin, "Optimization of test interval for ageing equipment: a multi-objective genetic algorithm
- approach", J. loss prev. process ind., vol. 24, no. 4, pp. 397-404, 2011. 12. Ivo Kljenak, Borut Mavko, "Simulation of containment thermalhydraulics in the Marviken Blowdown 16 experiment with ASTEC and CONTAIN codes", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1063-1070, 2011.
- 13. Boštjan Končar, C. Morel, S. Mimouni, L. Vyskocil, M. C. Galassi, "Computational fluid dynamics modeling of boiling bubbly flow for departure from nucleate boiling investigations", Multiph. sci. technol., vol. 23, no. 2/3, str. 165-222, 2011. [COBISS.SI-ID 25746471]
- 14. Boštjan Končar, Igor Simonovski, Martin Draksler, "Influence of multiple jet cooling on the heat transfer and thermal stresses in DEMO divertor cooling finger", Fusion eng. des., vol. 25, no. 2, pp. 537-548, 2011.
- 15. Andrej Prošek, "Uporaba grafičnega uporabniškega vmesnika za varnostno analizo poskusa ROSA/LSTF z zlomom v vroči veji", Elektrotehniški vestnik, vol. 78, no. 3, pp. 147-152, 2011.
- Andrej Prošek, Borut Mavko, "Animation model of Krško nuclear power plant for RELAP5 calculations", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1034-1046, 2011.
- 17. Igor Simonovski, Leon Cizelj, "Automatic parallel generation of finite element meshes for complex spatial structures", Comput. mater. sci., vol. 50, no. 5, pp. 1606-1618, 2011.
- 18. Igor Simonovski, Leon Cizelj, "Computational multiscale modeling of intergranular cracking", J. nucl. mater., vol. 414, no. 2, pp. 243-250, 2011.
- 19. Luka Štrubelj, Iztok Tiselj, "Two-fluid model with interface sharpening", Int. j. numer. methods eng., vol. 85, no. 5, pp. 575-590, 2011
- 20. Luka Štrubelj, Iztok Tiselj, "Numerical simulations of basic interfacial instabilities with incompressible two-fluid model", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, Nucl. Eng. Des., vol. 241, no. 4, pp. 1018-1023, 2011.
- 21. Mitja Uršič, Matjaž Leskovar, Borut Mavko, "Improved solidification influence modelling for Eulerian fuel-coolant interaction codes", In: Special issue on the International Conference Nuclear Energy for New

Europe 2009, Bled, Slovenija, *Nucl. Eng. Des.*, vol. 241, no. 4, pp. 1206-1216, 2011.

22. Andrija Volkanovski, Marko Čepin, "Implication of PSA uncertainties on risk-informed decision making", In: Special issue on the International Conference Nuclear Energy for New Europe 2009, Bled, Slovenija, *Nucl. Eng. Des.*, vol. 241, no. 4, pp. 1108-1113, 2011.

## **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

- 1. Leon Cizelj, Guy Roussel, "Reliability of degraded steam generator tubes", In: *Steam generator systems: operational reliability and efficiency*, Valentin Uchanin, ed., Rijeka, In-Tech, cop. 2011, pp. 117-142.
- 2. Matjaž Leskovar, "Simulation of ex-vessel steam explosion", In: *Nuclear power operation, safety and environment*, Pavel V. Tsvetkov, ed., Rijeka, InTech, cop. 2011, pp. 207-236.
- 3. Andrej Prošek, Matjaž Leskovar, "Application of fast Fourier transform for accuracy evaluation of thermal-hydraulic code calculation", In: *Fourier transforms - approach to scientific principles*, Goran S. Nikolić, ed., Rijeka, In-Tech, cop. 2011, pp. 447-468.

## PUBLISHED CONFERENCE PAPERS

#### **Invited Papers**

- 1. Andrej Prošek, Ovidiu-Adrian Berar, Borut Mavko, "Bethsy 9.1b test calculation with TRACE nad RELAP5", In: *Proceedings*, CAMP Meeting 2011, 27-29 April 2011, Bariloche, Argentina, [S. l., s. n.], 2011, 24 pp.
- 2. Andrej Prošek, Borut Mavko, Ovidiu-Adrian Berar, "Status of CAMP activities in Slovenia", In: *Proceedings*, CAMP Meeting 2011, 27-29 April 2011, Bariloche, Argentina, [S. l., s. n.], 2011, 24 pp.

#### **Regular** papers

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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 servicing of industrial radioactive sources and surveillance of the fuel management in NPP Krško.

In 2011 the reactor operated for 117 days. A total of 737 samples were irradiated including 676 in the rotary specimen rack and 61 in the pneumatic transfer system.

The reactor was mostly operated in a steady-state mode. There were no serious operational problems or events Head: influencing the nuclear or radiation safety. The reactor operators were performing regular maintenance inspections **Prof. Borut Smodiš** and activities in line with the annual plan.

In the Hot Cells Facility that was mainly used for the work with strong radioactive sources, the activities were mostly performed by the Department of Environmental Sciences and the Radiation Protection Unit. In 2011 the IJS staff carried out a training in radiochemistry and radioactivity measurements for the practitioners from the countries eligible under the JRC Enlargement & Integration Policy.

The reactor was mostly used for the neutron activation analysis. The reactor operated mainly for the needs of the Jožef Stefan Institute's Milan Čopič Nuclear Training Centre, for its education and research departments: the Environmental Sciences, the Reactor Physics, the Experimental Particle Physics and the Nanostructured Materials. The reactor was used for the following research:

- neutronics and reactor physics
- activation analysis
- neutron dosimetry and spectrometry
- neutron radiography
- activation of materials, nuclear waste and decommissioning
- irradiation of materials for fusion reactors.



Figure 1: View into the reactor core during the operation

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 about 20 scientific papers. Three young researchers performed their researches at the reactor.

In 2011 the following international courses on the safety of research reactors were carried out:

- 1. IAEERRI11: IAEA Group Fellowship Training, Programme on Research Reactors, 7-18 March 2011 4 participants
- 2. IAEERRI12: IAEA Group Fellowship Training, Programme on Research Reactors, 7-18 November 2011 5 participants
- 3. TJE T12: Nuclear Power Plant Technology, ICJT, 15 October 2010 11 April 2011 18 participants
- 4. THE T13: Nuclear Power Plant Technology, ICJT, 7 November 2011 2 April 2012 15 participants

Practical exercises in reactor physics and kinetics for the students of physics at Ljubljana University were preformed. The post graduate students of nuclear engineering attended some of these exercises as well. For these purposes the reactor operated for about 2 months. The reactor was used also for practical exercises within the training programme for the NPP Krško reactor operators. The exercises were prepared and carried out by the reactor personnel in co-operation with the Nuclear Training Centre and the Department of Reactor Physics.

In 2011 there were more than 50 short group visits to the reactor. The visitors were mainly foreign scientists, students and more than 30 groups of school children. Their total number was more than 900.

## INTERNATIONAL PROJECTS

- IAEA Fellowship for Mr Fahti M. Zubeir IAEA Fellow, LIB/10001, Pr. LIB/4/011 IAEA, Vienna, Austria Dache Veräch R. Ga. Da Badaiba La finar
- Darko Kavšek, B. Sc., Dr. Radojko Jaćimović
  Training in Radiochemistry and Radioactivity Measurements for Practitioners from Countries Eligible under the JRC Enlargement & Integration Policy C59072

European Commission, Joint Research Center JRC, Institute for Reference Materials and

## MENTORING

#### Ph. D. Thesis

1. Meleq Bahtijari, Radon in Kosovo (mentor Peter Stegnar; co-mentor Zahadin Shemsidini).

Measurements (IRMM), Geel, Belgium Prof. Borut Smodiš, Asst. Prof. Ljudmila Benedik

## NEW CONTRACTS

 Program of radioactivity monitoring around the Žirovski Vrh Uranium Mine during intermediate (five years) period after the final remediation of dumping grounds at Jazbec and Boršt, and the pit in the year 2011 RŽV, d. o. o. Prof. Borut Smodiš

M. Sc. Thesis

 Nejc Mekiš, Sacroiliac joint imaging : achieving dose reduction with PA projection (mentor Peter Stegnar; co-mentor Igor Kocijančič).

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- Thomas Breznik, Marko Gerbec, Borut Smodiš, "Task analysis and risk assessment of the transport of the radioactive material by road in the Republic Slovenia", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 8 pp., 2011.
- 3. Igor Lengar, Luka Snoj, "Benchmark evaluation of interacting aluminum cylinders containing uranyl fluoride solution", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 11 pp., 2011.
- 4. Stanko Manojlović, Andrej Trkov, Luka Snoj, Gašper Žerovnik, "Nuclear cross-section measurement analysis in the Californium-252 spectrum with the Monte Carlo method", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 8 pp.
- 5. Manca Podvratnik, Luka Snoj, Andrej Trkov, Gašper Žerovnik, "Calculations to support absolute thermal power calibration of the Slovenian TRIG Mark II reactor", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 9 pp.
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- 12. Marko Štrok, Petra Planinšek, Borut Smodiš, "Content of natural radionuclides in sediments in the vicinicy of a former uranium mine", In: *Zbornik radova VIII. simpozija Hrvatskog društva za zaščitu od zračenja: HDZZ - CRPA: Zagreb 2011*, Ines Krajcar Bronić, ed., Zagreb, Hrvatsko društvo za zaščitu od zračenja, 2011, pp. 431-436.
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- 1. Ljudmila Benedik, Vekoslava Stibilj, Borut Smodiš, Marko Štrok, Training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC enlargement&integration policy: Training Manual, Reactor Center, November 21- December 2, 2011, Ljubljana.
- 2. Borut Smodiš, Introduction to Sr-89/90 and H-3: Training in radiochemistry and radioactivity measurements for practitioners from the countries eligible under the JRC enlargement and integration policy, Ljubljana, Ljubljana, 2011.
- 3. Borut Smodiš, Radioactivity and nuclear methods for studying processes: third-level study programme "Ecotechnology", autumn semester 2011/2012, Ljubljana, Ljubljana, 2011.
- Borut Smodiš, Radioaktivnost, radionuklidi, detekcija in meritve, radiokemija, tritij: Storitve kemičnega in biološkega laboratorija, Ministrstvo za obrambo RS, 2011, Ljubljana, 2011.
- Borut Smodiš, Ravnanje z odpadki; modul; radioaktivni odpadki: Bolonjski študij prve stopnje, leto 2011/2012, Nova Gorica, Fakulteta za znanosti o okolju, 2011.
- 6. Borut Smodiš, Research reactor utilisation: East European research reactors inciative, Group felowship training course Vienna-Ljubljana-Prague, Ljubljana, 2011.

## 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.

## STAFF

## Technical officers

- 1. Vladimir Alkalaj, M. Sc., Head Technical and administrative staff
- 2. Ivan Ivanjko
- Matjaž Levstek
- 4. Mark Martinec, B. Sc.
- 5. Janez Srakar
- 6. Matej Wedam



Vladimir Alkalaj, M. Sc.\*



Figure 1: JSI connectivity structure



Figure 2: Layout of JSI communication network \*Photo by Sašo Rebolj Playboy

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1. Tomaž Erjavec, Jan Jona Javoršek, Matija Ogrin, Petra Vide Ogrin, "Od biografskega leksikona do znanstvenokritične izdaje: vprašanje trajnosti elektronskih besedil", *Knjižnica (Tisk. izd.)*, vol. 55, no. 1, pp. 103-114, 2011.

Matija Ogrin, Jan Jona Javoršek, Tomaž Erjavec, "Rokopisi slovenskega slovstva baročne in razsvetljenske dobe: predmet več ved in metod", In: *Meddisciplinarnost v slovenistiki*, (Obdobja, Simpozij, = Symposium, 30), Simona Kranjc, ed., 1. natis, Ljubljana, Znanstvena založba Filozofske fakultete, 2011, pp. 337-341.

## 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.

We supplement our comprehensive print collection of core journals with the electronic editions, offered through our WWW site. We subscribe to the electronic collections offered by ScienceDirect, Springer Link, IEEExplore, Stanford HighWire Press, ACS online editions, AIP electronic editions, IoP online journals, Wiley Interscience. We provide access to the SCOPUS, INSPEC, Crossfire Beilstein, and Web of Science databases, and the Dialog on-line database services.

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.



## INTERNATIONAL PROJECTS

Slovenian National Open Access Web Site OPENACCESS.SI 1. Contract dtd, 4.4.2011 Rebecca Neilson, Stichting eIFL.net, Utrecht, The Netherlands Dr. Luka Šušteršič

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- Katarina Modic, B. Sc.
- 6. Joško Per
- Alenka Sosič, B. Sc.
- Jože Škulj
- Slavka Šmuc, B. Sc. 10. Branka Štrancar
- 11. Nada Tratnik
- 12. Saša Žnidar

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# **ENERGY EFFICIENCY CENTRE**

# EEC

The basic activities of the Energy Efficiency Centre are related to efficient energy use, long-term energy planning and the reduction of greenhouse-gas emissions. The Centre is a focal point for the collection and transfer of energy-efficiency technologies to the energy users, the state, the energyservice and equipment providers, and other interested parties. At the same time it deals with the environmental effects of energy use and energy conversion. The most significant part of the EEC's activities is thus the cooperation with state institutions in the preparation of strategic documents and legislation relating to the efficient energy use, energy planning, distributed electricity production, and emission trading. The EEC also continues to be strongly connected, through its consulting and training activities, with industrial companies and other institutions.

#### **Energy and the environment**

In 2011 the EEC was also intensely involved in the preparation of the key development strategic documents relating to energy planning and greenhouse-gas-emission reduction.

Head.

For the Ministry of the Economy, strategic studies and a proposal for the new National Energy Programme Stane Merše, M. Sc. (NEP) were prepared and a broad public discussion about the documents was carried out, representing a demanding challenge and the greatest professional task the EEC has ever assumed. The preparation of the strategic studies and the quantitative analysis needed for the preparation and evaluation of the sub-programmes in all key fields required a complete update of all the developed models and software tools, especially the Referential Energy Environment Model of Slovenia (REES-SLO2) that was done in the new MESAP environment.

The accepted EU climate-energy package has set, for Slovenia, new ambitious goals regarding an increase in the energy efficiency, exploitation of renewables and the reduction of greenhouse-gas emissions. An efficient energy use is a priority in this area. In line with the requirements of the European Commission and the Energy Service Directive (2006/32/ES), the EEC, together with the Ministry of the Economy, carried out the Second National Action Plan for Energy Efficiency for the Period 2011 - 2016. We prepared the evaluation methodologies for implementing the energyefficiency measures that present the key tools for achieving the set goals. The preparation of the methodologies was included in a broader process of preparing the harmonized evaluation methodologies carried out at the EU level, where the cooperation in the framework of "Concerted Action - Energy Service Directive (CA-ESD)" was in progress.

In the field of greenhouse-gas-emission reduction, the Centre carried out new projections of greenhouse-gas emissions and prepared a report for the

European Commission, and new projections of the pollutant emissions from the NEC directive for the Ministry of the Environment. The Centre also cooperated with the Governmental Office for Climate Changes in the preparation for the negotiation about Slovenia's starting points as regards the new goals of the EU climate policy until 2020 and 2050, as well as in the preparation of Slovenia's climate strategy until 2050.

In 2011 the Centre also continued to be active as the state referential center for energy by preparing a list of indicators relating to energy and environment.

In 2011 a successful cooperation with the Municipality of Ljubljana (MOL) continued, as we performed a study, supported by Siemens, called Sustainable Municipal Infrastructure - Ljubljana - a View up to 2050 that, on the basis of an analysis of two scenarios of the CO<sub>2</sub>-emission reduction (-50% and -80%) represents a vision of a sustainable city development up to 2050. The Center also prepared an investment programme for the energy renovation of public buildings owned by MOL and a tender for

technical assistance ELENA, which will enable the financing of the investments with the EIB funds including the enterprises for carrying out the energy services and an energy contracting model.



Figure 1: Movement of the greenhouse-gas emissions by sector for the period 1986-2009 and an assessment of the effect of the National Energy Programme until 2030 within the basic scenario of the energy development.

With its research-and-development work, the Energy Efficiency Centre contributes significantly to the preparation of the key Slovenian documents in the fields of energy development, energy efficiency, renewables exploitation and the transition of Slovenia to a low-carbon society. By organising training activities and supporting industry, the Centre promotes competitiveness and development restructuring.

#### Promotion of an efficient energy use and energy consulting

With respect to the promotion of an efficient energy use and energy consulting in industry and institutions, the Centre continued with its training activities, so that the fourth cycle of the energy-managers training was successfully



Figure 2: Decrease of energy costs and achieved savings – Second national action plan for energy efficiency for the period 2011-2016.

concluded within the European programme EUREM. Furthermore, in the autumn the fifth cycle of the training was started. Due to a very positive reaction from the participants and their interest, 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. A great acknowledgement of our successful work is the European Energy Manager of the Year diploma for small enterprises awarded to Mr. Janez Štaudohar from Petrol for the project Planina Kranj and to Andrej Novak from the Uralita company for the project on the energy-use optimization in the process of polimerization.

In 2011 the Center of Energy Efficiency carried out several consulting tasks in industry and performed a series of energy audits of enterprises and institutions to reduce the consumption and the costs for energy and emissions. The largest clients include Luka Koper, Municipality of Ljubljana, Borzen – Support Center, Tanin Sevnica, etc.

The Centre also prepared the conference programme and was involved in the organisation of the twelfth Slovenian conference of energy managers called "Energy Managers Days", the annual meeting of energy managers with

more than 200 participants. This confirms the quality and the public profile of the Centre's professional work. In 2011 the Centre prepared electronic issuing of the Energy Efficiency Newsletter for the Ministry of the Economy. Individual EEC experts published numerous articles in magazines and public media as well as taking part in radio and television broadcasts.

#### International cooperation

In 2011 the EEC carried out as many as 10 international projects, financed by the European Union resources in the framework of the 7FP and the European Commission programme "Intelligent Energy for Europe", as well as MEDITERAN and South East Europe.

Projects covered the activities in the following fields:

- Promotion and development of new energy services project Good Practice Examples of Changes in Energy Services (ChangeBest)
- Development and provision of energy contracting and advanced energy services project European Energy Service Initiative (EESI)
- Monitoring the execution of the Directive on Cogeneration project Cogeneration Observatory and Dissemination Europe (CODE)
- Compiling and elaboration of the current data on the use of renewable energy sources EurObserv`ER Barometer
- Monitoring the indicators of energy use and energy efficiency in the EU project Monitoring of Energy Demand Trends and Energy Efficiency in the EU (ODYSSEE MURE EU-27)
- Introduction of intelligent systems of energy management in the public sector project Intelligent Information Systems for Monitoring and Verification of Energy Management in Cities (ISEMIC)
- Energy efficiency in households with low income in the Mediterranean with an emphasis on the introduction
  of smart measurements project Energy Efficiency in Low-Income Housing in the Mediterranean (Elih-MED)
- Inclusion of the criteria for energy efficiency in the public tenders project Upgrading of Energy Efficient Public Procurement for a Balanced Economic Growth of the SEE Area (EFFECT)
- Increase of energy efficiency in services (hospitals) with an introduction of energy management and the provision of measures with low investment costs – project Re-Commissioning – Raising Energy Performance in Existing Non-Residential Buildings (Re-Co)
- Innovative systems of energy-use monitoring and management in industry to support energy-use reduction and emission trading – project Context Sensitive Monitoring of Energy Consumption to Support Energy Savings and Emissions Trading in Industry (Life Saver)

The above projects required cooperation with research and development 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.

## Some outstanding achievements in 2011

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).



Figure 3: Award of EUREM certificates – European Energy Manager – to the fourth generation of EUREM training participants.

- 2. Establishment of energy managers training in the framework of the European project EUREM and professional support to industry and other institutions by carrying out energy audits, feasibility studies and other consulting (Goodyear, Cinkarna Celje, Litostroj, TE-TOL, Luka Koper, etc.).
- 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, external costs in energy, exploitation of wood biomass and others.

## Organization of conferences, congress and meetings

- 1. Energy Managers Days 2011 13th Meeting of Energy Managers of Slovenia, Portorož, 11.- 12.4.2011
- 2. Workshop on the project Cogeneration Observatory and Dissemination Europe (CODE), Ljubljana, 25.1.2011
- Monitoring of EU and national energy efficiency targets (ODYSSEE-MURE 2010 2012), Ljubljana 31.3.
   1.4.2011
- 4. European Energy Manager Training, Ljubljana, 19.1.- 21.1., 9.3.- 11.3., 11.5.- 13.5. and 17.6.2011
- 5. Workshop on the project ChangeBest and EESI, Ljubljana, 15.6.2011

## INTERNATIONAL PROJECTS

- Context Sensitive Monitoring of Energy Consumption to Support Energy Savings and 1. Emission Trading in Industry LifeSaver 7. FP, 287652 EC; Rui Neves-Silva, UNINOVA - Instituto de Desenvolvimento de Novas, Monte Caparica, Portugal Boris Sučić, M. Sc Re-Comissioning-Raising Energy Performance in Existing Non-Residential Buildings Re-Co IEE Programme IEE/10/328/SI2.58942 EC; Grazer Energie Agentur GmbH, GEA, Gesellshaft mit beschränkter Haftung, Graz, Austria Barbara Petelin Visočnik, M. Sc. Monitoring of EU and National Energy Efficiency Targets **ODYSSEE MURE 2010** IEE Programme IEE/09/801/SI2.558254 EC; Didier Bosseboeuf, Agence De l'Environnement et de la Maitrise de l'Energie (ADEME), Angers, France Dr. Fouad Al-Mansour The EurObser'ER Barometer Backs the New RES Directive EurObserv'ER 2020 **IEE Programme** IEE/09/737/SI2.558317 EC; Observatoire des Energies Renouvelables (Observ´ER), Paris, France Dr. Fouad Al-Mansour European Energy Service Initiative EESI IEE Programme IEE/08/581/SI2.528408 EC; Michael Geissler, Berliner Energiagentur GmbH (BEA), Berlin, Germany Damir Staničić, M. Sc.
- Good Practice Examples of Changes in Energy Service Business, Strategies and 6. Supportive Policies and Measures in the Course of the Implementation of Directive 2006/32/EC ChangeBest IEE Programme IEE/08/434/SI2.528383 EC; Wuppertal Institut für Klima, Umwelt, Wuppertal, Germany Barbara Petelin Visočnik, M. Sc. 7. Cogeneration Observatory and Dissemination Europe C.O.D.E IEE Programme IEE/07/564/SI2.499462 EC; COGEN EUROPE, Brussels, Belgium Stane Merše, M. Sc. Concerted Action Supporting Transposition and Implementation of Directive 2006/32/8 EC of the Council CA ESD IEE Programme IEE/CA/08/001/SI2.503473 EC; Rob Boeree, SenterNovem, Sittard, The Netherlands Damir Staničić, M. Sc. 9. Intelligent Information System for Monitoring and Verification of Energy Management in Cities ISEMIC SEE-ERA.NET Plus ERA 163/01 EC; Prof. Željko Tomšić, University of Zagreb, Faculty of Electrical Engineering and Computing, Department of Power Systems, Zagreb, Croatia Boris Sučić, M. Sc. 10. Energy Efficiency in Low-Income Housing in the Mediterranea ELIH-Med MED Programme IS-MED10-029

EC; Joint Technical Secretariat, MED Programme, Conseil Regional Provence-Alpes-Cote d'Azur, Marseille, France; Eng. Marco Casagni, National Agency for New Technologies, Energy and Sustainable Economic Development, Rome, Italy Aleš Podgornik, M. Sc.

11. Upgrading of Energy Efficient Public Procurement for a Balanced Economic Growth of SEE

Area within the South East Europe Transnational Cooperation Programme (SEE)  $\ensuremath{\mathsf{EFFECT}}$ 

South East Europe Programme

SEE/B/0022/2.4/X

ARAEN - Abruzzo Regional Energy Agency, Pescara, Italy

Polona Lah, B. Sc.

 Expert Training under the Programme "Role of Energy Managers in the Process of the Improvement of Energy Efficiency in Public Sector", 20. - 21. 10. 2011, for the Managers from the Kula, Vojvodina, Serbia; held in Ljubljana, Slovenia Ugovor, 21.10.2011

Nevena Vasic, Barcino Tours d.o.o., Niš, Serbia

Boris Sučić, M. Sc.

## R & D GRANTS AND CONTRACTS

#### 1. Slovenia - Low carbon society Andreja Urbančič, M. Sc

 "Environmental footprint of agriculture and food processing industry and technological measures for its lowering in the future" Dr. Fouad Al-mansour

## RESEARCH PROGRAM

1. Modelling and environmental impact assessment of processes and energy technologies Prof. Borut Smodiš

## VISITORS FROM ABROAD

- 1. Louis Charles Arrive, French Embassy in Slovenia, Ljubljana, Slovenia, 15.3.2011
- 2. Didier Bosseboeuf, senior expert, ADEME, Paris, France, 31.3. 1.4.2011
- 3. Bruno Lapillonne, director, ENERDATA, Paris, France, 31.3. 1.4.2011
- 4. dr. Piet Boonekamp, senior expert, ECN, Amsterdam, the Netherlands, 31.3. 1.4.2011
- 5. Iatridis Minas, expert, CRES, Athens, Greece, 31.3. 1.4.2011
- 6. Wolfgang Eichhammer, senior expert, Fraunhofer ISI, Germany, 31.3. 1.4.2011

## NEW CONTRACTS

- Sustainable Municipal Infrastructure Ljubljana View up to 2030 Siemens d. o. o. Boris Sučić, M. Sc.
- Continuation of Activities to Support the Preparation of the National Energy Programme Ministry of Economic Development and Technology

Ministry of Economic Development and Technology Andreja Urbančič, M. Sc.

3. Professional cooperation in current fields of gaining support for electricity produced from RES and CHP

Termoelektrarna Toplarna Ljubljana, d. o. o. Stane Merše, M. Sc.

 Strategic studies for the national action plan for energy efficiency for the period from 2011 to 2016

Ministry of Economic Development and Technology Damir Staničić, M. Sc.

- Professional help and cooperation in the execution of the EU programme project CLIMEPORT – component WP Luka Koper d. d.
- Asst. Prof. Marko Pečkaj
- Updating of indicators environment energy within tasks of the national referential centre for energy in the year 2012 Ministry of the Environment and Spatial Planning
- Matjaž Česen, B. Sc. 7 Energy Managers Days 2011
- . Energy Managers Days 2011 Časnik Finance
- Stane Merše, M. Sc.
- Stane Merse, M. Sc.
   Energy balances of RS for the year 2011 Ministry of Economic Development and Technology
- Elaboration of the investment programme of energy renovation of public buildings
- MOL ELENA Energetika Ljubljana d.o.o. Stane Merše, M. Sc.
- 7. Lea Gynther, expert, Motiva Oy, Helsinki, Finland, 31.3. 1.4.2011
- Zorica Ačanski Omerović, Development Agency of the Municipality Kula, Kula, Serbia, 20. – 21.10.2011
- 9. Nikola Vujović, Directorate for the Construction of Vrbas, Serbia, 20. 21.10.2011
- 10. Vera Žarković, Municipality of Bačka Palanka, Serbia, 20. 21.10.2011

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## Researchers

- 1. Dr. Fouad Al-Mansour
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- Damir Staničić, M. Sc.
   Andreja Urbančič, M. Sc.
- 5. Andreja Urbancic, M Postgraduates
- 6. Anja Kostevšek\*'
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- 16. Matevž Pušnik, B. Sc.
- 17. Igor Ribič
- 18. Milan Simončič, B. Sc., retired 01.04.11

Note:

\*\* postgraduate financed by industry
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- Journal of energy technology, iss. 5, vol. 4, pp. 49-63, 2011. 3. Stane Merše, "Projekt CODE", Učin. energ., april, 2011.
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#### **Regular** papers

- Djani Brečević, Saša Jamšek, Enisa Rojnik, Boris Sučić, "Razvoj elektroenergetskega omrežja Republike Slovenije v kontekstu doseganja ciljev energetske politike EU", In: Deseta konferenca slovenskih elektroenergetikov, Ljubljana, 30. maj - 1. junij 2010, [Ljubljana, Slovensko društvo elektroenergetikov CIGRÉ - CIRED], 2010 [i. e. 2011], pp. 1-5.
- Aleš Podgornik, Damir Staničić, Boris Sučić, Andreja Urbančič, "Analysis of Slovenian wind energy potential", In: *DEMSEE 2011*, 6th International Workshop on Deregulated Electricity Market Issues in South-Eastern Europe, 20.-21. September 2011, Bled, Slovenia, Urban Rudež, ed., Ljubljana, Založba FE in FRI, cop. 2011, 6 pp., 2011.
- Aleš Podgornik, Damir Staničić, Boris Sučić, Andreja Urbančič, "Vloga sektorja elektroenergetike pri doseganju slovenskih ciljev podnebno energetskega paketa EU", In: *Deseta konferenca slovenskih elektroenergetikov, Ljubljana, 30. maj - 1. junij 2010*, [Ljubljana, Slovensko društvo elektroenergetikov CIGRÉ - CIRED], 2010 [i. e. 2011], 7 pp.

- 4. Matevž Pušnik, Boris Sučić, Stane Merše, Matjaž Česen, Andreja Urbančič, "Role of the national energy system modelling in the process of the policy development", In: *Conference proceedings*, 6th Dubrovnik Conference on Sustainable Development of Energy, Water and Environment Systems, September 25 - October 29, 2011, Dubrovnik, Croatia, [S. l., s. n.], 2011, 14 pp.
- Damir Staničić, Boris Sučić, Aleš Podgornik, Andreja Urbančič, "Challenges of the new Slovenian renewable energy action plan - path toward the low-carbon economy", In: *Conference proceedings*, 6th Dubrovnik Conference on Sustainable Development of Energy, Water and Environment Systems, September 25 - October 29, 2011, Dubrovnik, Croatia, [S. l., s. n.], 2011, 11 pp., 2011.
   Boris Sučić, Matjaž Česen, Damir Staničić, Stane Merše, Andreja
- 6. Boris Sučić, Matjaž Česen, Damir Staničić, Stane Merše, Andreja Urbančič, Matevž Pušnik, Peter Bevk, "Aktivno upravljanje z energijo kot prvi korak prehoda Ljubljane v nizkoogljično prestolnico", In: Dajmo prednost energetski učinkovitosti!: zbornik, Barbara Petelin-Visočnik, ed., Stane Merše, ed., Ljubljana, Časnik Finance, 2011, 16 pp., 2011.
- 7. Boris Sučić, Andreja Urbančič, Polona Lah, Zvonko Košnjek, "Electricity production and prices - case study Slovenia, trends up to 2030", In: *DEMSEE 2011*, 6th International Workshop on Deregulated Electricity Market Issues in South-Eastern Europe, 20.-21. September 2011, Bled, Slovenia, Urban Rudež, ed., Ljubljana, Založba FE in FRI, cop. 2011, 5 pp., 2011.
- Andreja Urbančič, Stane Merše, Boris Sučić, Damir Staničić, Polona Lah, Matjaž Česen, Matevž Pušnik, Aleš Podgornik, Zvonko Košnjek, Miroslav Bugeza, Djani Brečević, Saša Jamšek, Andrej Bučar, "Nacionalni energetski program: strokovne podlage za odločanje", In: Deseta konferenca slovenskih elektroenergetikov, Ljubljana, 30. maj - 1. junij 2010, [Ljubljana, Slovensko društvo elektroenergetikov CIGRÉ -CIRED], 2010 [i. e. 2011], 7 pp.

#### **RESEARCH MONOGRAPH**

1. Stane Merše, Barbara Petelin-Visočnik, F. Riddoch, S. Craenen, Paul D. Gardiner, T. Rotheray, N. Butterworth, C. Theofylaktos, M. Reijalt, A. Fontana, *Cogeneration case studies handbook: code project*, Ljubljana, Jožef Stefan Institute, Energy Efficiency Centre, 2011.

## CENTRE FOR ELECTRON MICROSCOPY

## CEM

The Center for Electron Microscopy (CEM) has the function of a supporting infrastructure center at the JSI that 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 analysis 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 that belongs to the Center of Excellence NiN and in 2009 a newly installed field-emission scanning electron microscope JSM-7600F, which was a joint purchase of 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 JEM-2010F, ADF detector on JEM-2010F and EBSD system on 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 analysis on the micro-scale is also possible. Since only a few µm<sup>3</sup> of the material is nonde-structively 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. The JEM-2010F is a state-of-the-art TEM/STEM microscope with a FEG (field-emission gun) electron source and with 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 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 analyses (EDS, EELS). The CEM also comprises the equipment for SEM and TEM specimen preparation, which is the first starting step for all electron-microscopy observation procedures. Particularly important are high- and low-energy ion-millers, which enable the preparation of thin foils that are transparent for high-energy electrons.

The analytical work that is performed on the CEM equipment varies, concerning both the investigated materials and/or the used electron microscopy techniques. While scanning electron microscopy is used mainly for microstructural characterization and the 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 analyses of grain boundaries is especially important, since it is known that the final physical properties to a great extent depend on the structure and chemistry of the 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, one on the main tasks is to attain the maximum possible operating time of the microscopes. This complex and expensive equipment needs regular daily maintenance, apart from 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 1: Cross-sectional and surface FE-SEM images of the (K0.5Na0.5) NbO3 thin films on Pt(111)/TiO2/SiO2/Si substrates from the acetatealkoxide-based precursor sols with the (a) stoichiometric composition and with (b) 5 mole % or (c) 10 mole % excess of potassium acetate. Electronic Ceramics: A. Kupec



Figure 2: TEM bright-field micrograph of the TiN layer on the surface of a titanium alloy. The TiN coating was prepared by nitridation of the metal at elevated temperatures in an ammonia atmosphere. Engineering Ceramics: I. Pribošič



Figure 3: The experimental HRTEM image detail from Ba-hexaferrite nanoparticle close to the [120] zone axis with two superimposed calculated images and the corresponding atomic models. Image was acquired with the JEM-2010F. The HRTEM image analysis showed that the intensity variations in the experimental image are extremely sensitive to defocus value, and thus, the position of heavy the Ba atoms in the nanoparticle's structure cannot be determined with a high level of confidence. Nanostructured Materials: S. Šturm



Figure 4: Scanning electron microscopy image and transmission electron microscopy image of a dendrite hexagonal platelet particle of magnetic perovskite LaSrMnO3. Synthesis of Materials: SEM image: S. Ovtar, TEM image: D. Makovec





50 nm

PEM+Ag<sub>2</sub>O NPs



Figure 5: (a) Polyelectrolyte multilayer-titanate nanobelts (PEM/Ti-NBs) composite, (b) Ag20 nanoparticles within the PEM assembled on the surface of Ti-NBs and (c) Ag nanoparticles/Ti-NBs 1D nanocomposite. Advanced Materials: I. Bračko

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 2011 the centre was active in several European projects from FP7 PASCAL2 (Pattern Analysis, Statistical Modelling and Computational Learning 2), ACTIVE (Enabling the Knowledge Powered Enterprise), COIN (COllaboration and INteroperability for networked enterprises) and EURIDICE (European Inter-Disciplinary Research on Intelligent Cargo for Efficient, Safe and Environment-friendly Logistics), 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 Mitja Jermol, M. Sc. Network of Excellence on Large-Scale Data Management ) and e-LICO (An e-Laboratory for Interdisciplinary Collaborative Research in Data Mining and Data-Intensive Science) and TRANSLECTURES (Transcription and Translation of Video Lectures).



Head

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, automatization 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 14,577 recorded tutorials from different scientific events and is visited daily by an average of 8000 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 scholars and scientists at the most important and prominent events. For the fourth year 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 and CMU, as well as with the European CERN and ETH from Zurich.

The centre also operates a web portal http://www.ist-world.org that offers services for automatic data collection and an analysis of the European research. The user can perform several simple and complex analyses, predictions and detect trends in research. The database currently contains data from about 100,000 research organizations, 42,500 research projects and around 2 million experts from Europe. This is an exceptional web service that is being visited daily by an average of 5,000 unique visitors.

In 2011 we organized the 6<sup>th</sup> Student Competition in Computer Science, attended by 139 students from Slovenian secondary schools and a video workshop for selected participants from the 6<sup>th</sup> Student Competition in Computer Science. We have also organized four project meetings for different EU projects (ACTIVE, ALERT, RENDER and MULTILINGUAL WEB) and an international workshop for the EU project GENDERA "Encouraging gender equality policy". In the autumn we organized a "Winter School on Knowledge Technologies for Complex Business Environments", which was attended by 31 experts.

Our role in the FP7 integrated projects COIN "COllaboration and INteroperability for networked enterprises, EURIDICE" European Inter-Disciplinary Research on Intelligent Cargo for Efficient, Safe and Environment-friendly Logistics, ACTIVE "Enabling the Knowledge Powered Enterprise" and in three net- competition in computer science

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 a second one is http://www.ist-world.org, which offers services for automatic data collection and analysis of the European research.



Figure 1: Poster of the 6th Student

For the fourth year the portal http:// videolectures.net/ collaborates with Massachusetts Institute of Technology (MIT), YALE, University of California - Berkeley, University of Ljubljana, and with European **Organization for Nuclear Research - CERN.** 

works of excellence PASCAL2, PLANET DATA and METANET was the support and coordination of all educational and dissemination activities as well as knowledge transfer.

#### Organization of conferences, congress and meetings

- Final review meeting of the EU project ACTIVE, Ljubljana, 22.3.-25.3.2011 1.
- 2. 6th Student competition in computer science, Ljubljana, 26.3.2011
- Project meeting of the EU project ALERT, Bled, 11.4.-12.4.2011 3.
- Project meeting of the EU project RENDER, Ljubljana, 19.4.-20.4.2011 4.
- Video workshop for students, Ljubljana, 21. 5.2011 5.
- 6. Project meeting of the EU project MULTILINGUAL WEB, Bled, 7.6.-8.6.2011
- Winter School on Knowledge Technologies for Complex Business Environments, Ljubljana, 28.11.-2.12.2011 7.
- Project meeting of the EU project GENDERA, Ljubljana, 12.12.2011 8.

### INTERNATIONAL PROJECTS

1. Transcription and Translation of Video Lectures transLectures

7. FP, 287755

- EC; Alfons Juan, Universitat Politenica de Valencia, Valencia, Spain Mitja Jermol, M. Sc., Prof. Dunja Mladenič, Marko Grobelnik
- e-Laboratory for Collaborative Interdisciplinary Research in Data Mining and Data Intensive Sciences
- e-LICO
- 7 FP 257680

EC; Dr. Mélanie Hilario, Universite de Geneve, Carouge, Switzerland Mitja Jermol, M. Sc., Prof. Nada Lavrač, Asst. Prof. Martin Žnidaršič

- Active Support and Real-time Coordination based on Event Processing in Open Source 3. Software Development ALERT
  - 7. FP. 258098
  - EC; Dr. Ljiljana Stojanovic, Forschungszentrum Informatik an der Universität Karlsruhe, Karlsruhe, Germany
  - Mitja Jermol, M. Sc., Prof. Dunja Mladenić, Marko Grobelnik
- PlanetData 4.
  - PlanetData 7. FP
  - 257641

EC; Dieter Fensel, Universitaet Innsbruck, Innsbruck, Austria Mitja Jermol, M. Sc., Marko Grobelnik, Prof. Dunja Mladenić, Asst. Prof. Mihael Mohorčič

- 5. Reflecting Knowledge Diversity
  - RENDER
  - 7. FP
  - 257790

EC; Hartmut Schmeck, Karlsruhe Institute of Technology, Karlsruhe, Germany Mitja Jermol, M. Sc., Prof. Dunja Mladenić, Marko Grobelnik, Dr. Špela Stres

- Gender Debate in the European Research Area
- GENDERA

7. FP

7.

244499

EC; Dr. Dora Groo, Hungarian Science and Technology Foundation, Tudomanyos Es Technologiai Alapitvany, Budapest, Hungary Mitia Jermol, M. Sc., Prof. Dunia Mladenić

- Technologies for the Multilingual European Information Society
- MetaNet

7 FP 249119

EC: Dr. Stefhan Busemann, DFKI - German Research Center for Artificial Intelligence. Saarbrücken, Germany

Mitja Jermol, M. Sc., Marko Grobelnik, Prof. Dunja Mladenić

### VISITORS FROM ABROAD

- Ugo Negretto, ENICMA GmbH, Germany, 6.1.-7.1.2011 1.
- 2. Ugo Negretto, ENICMA GmbH, Germany, 8.3.-11.3.2011
- 3. Ugo Negretto, ENICMA GmbH, Germany, 22.3.-23.3.2011
- 4. Peter Laing, FIR-Research Institute for Operations Management, Aachen, Germany, 15.4.2011

- 8. Environmental Services Infrastructures with Ontologies ENVISION
  - 7. FP, 249120

EC; Bjorn Skjellaug, Arne J. Berre, Stiftelsen Sintef, Trondheiim, Norway

- Mitja Jermol, M. Sc., Prof. Dunja Mladenić, Miha Grčar, B. Sc., Prof. Nada Lavrač European Inter-Disciplinary Research on Intelligent Cargo for Efficient, Safe and
- Environment friendly Logistics EURIDICE
- 7 FP 216271
- EC; Dr. Paolo Paganelli, INSIEL Informatica per il Sistema Degli Enti Locali s.p.a, Trieste, Italy
- Mitja Jermol, M. Sc., Marko Grobelnik, Prof. Dunja Mladenić, Dr. Špela Stres
- 10. Enabling the Knowledge Powered Enterprise ACTIVE
  - 7. FP, 215040

EC; Dr. Paul Warren, British Telecommunications plc, London, Great Britain Mitja Jermol, M. Sc., Marko Grobelnik, Prof. Dunja Mladenić, Asst. Prof. Mihael Mohorčič

- 11. Pattern Analysis, Statistical Modelling and Computational Learning 2 PASCAL 2
  - 7. FP, 216886

EC; Prof. John Shawe-Taylor, University of Southampton, Highfield, Southampton, Great Britain

- Mitja Jermol, M. Sc., Prof. Dunja Mladenić, Marko Grobelnik
- 12. Collaboration and INteroperability for networked enterprises
- COIN 7. FP, 216256

EC; Dr. Claudia Guglielmina, TXT e-Solutions Spa, Milano, Italy

- Mitja Jermol, M. Sc., Prof. Dunja Mladenić, Marko Grobelnik
- 13. Opencast Matterhorn Project

00006855, Amendment no. 1, 00007260 University of California, Berkeley, Berkeley, CA, USA Mitja Jermol, M. Sc.

### NEW CONTRACT

- Agreement on cooperation in obtaining information from the sphere of international R & D environment in the defense sector AC/323 NATO RTO Ministry of Defence Mitja Jermol, M. Sc
- 5 Matthias Deindl, FIR-Research Institute for Operations Management, Aachen, Germany, 15.4.2011
- Marcel Scheibmayer, FIR-Research Institute for Operations Management, Aachen, 6. Germany, 15.4.2011
- Colin de la Higuera, Nantes University, France, 1.9.2011

Jean-Paul Calbimonte - Technical University of Madrid, Spain, 28.11.–2.12.2011
 Ugo Negretto - ENICMA GmbH, Germany, 28.11.–2.12.2011

16. Roland Stühmer - FZI Forschungszentrum Informatik, Germany, 28.11.-2.12.2011

- Ugo Negretto, ENICMA GmbH, Germany, 13.10.-14.10.2011
   Michael Witbrock Cycorp, Vice President of Research, USA, 28.11.-2.12.2011
- 10. Abraham B. Hsuan Irwin & Hsuan LLP, USA, 28.11.-2.12.2011
- Kostas Kalaboukas SingularLogic, Greece, 28.11.–2.12.2011
   Günter Ladwig AIFB, Karlsruhe Institute of Technology, Germany, 28.11.–2.12.2011,
- 13. Steffen Stadtmueller AIFB, KSRI, Karlsruhe Institute of Technology, Germany, 28.11. - 2.12.2011

### STAFF

#### **Technical officers**

- 1. Mitja Jermol, M. Sc., Head
- 2. Davor Orlić, B. Sc.
- Marjana Plukavec, B. Sc. 3.
- 4. Špela Sitar, B. Sc.

## BIBLIOGRAPHY

#### PUBLISHED CONFERENCE PAPERS

#### **Regular** paper

1. Mario Karlovčec, Dunja Mladenić, Marko Grobelnik, Mitja Jermol, "Visualizations of Slovenian scientific community", In: Zbornik 14. mednarodne multikonference Informacijska družba - IS 2011, 10.-14. oktober 2011: zvezek A: volume A, (Informacijska družba), Marko Bohanec, ed., Matjaž Gams, ed., Dunja Mladenić, ed., Marko Grobelnik, ed., Marjan Heričko, ed., Urban Kordeš, ed., Olga Markič, ed., Jadran Lenarčič, ed., Leon Žlajpah, ed., Andrej Gams, ed., Vladimir Fomichov,

17. Michele Sesana - TXT e-solutions, Italy, 28.11.-2.12.2011 18. Konstantin Hristov - FAVIT Network Ltd, Bulgaria, 28.11.-2.12.2011

#### Technical and administrative staff

- 5. Monika Kropej, B. Sc.
- 6 Sebastjan Mislej

ed., Olga S. Fomichova, ed., Andrej Brodnik, ed., Rok Sosič, ed., Vladislav Rajkovič, ed., Tanja Urbančič, ed., Mojca Bernik, ed., Ljubljana, Institut Jožef Stefan, 2011, pp. 129-132.

#### TEXTBOOKS AND LECTURE NOTES

- 1. Davor Orlič, Mitja Jermol, D12.4.2 Final training events report, Ljubljana, Jožef Stefan Institute, 2011.
- 2. Davor Orlič, Mitja Jermol, D6.2 Open training infrastructure, Ljubljana, Jožef Stefan Institute, 2011.

# MILAN ČOPIČ NUCLEAR TRAINING CENTRE

#### 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. Due to the change of generations in NPP Krško, this training has been very intensive in recent years. The most important is the Nuclear technology course, which is the initial training of future control-room operators. There were two courses in the calendar year 2011: the first started in the fall of 2010 and ended in the spring of 2011, and the second started in the fall of 2011 and will end in the spring of 2012. In addition, two courses Basics of nuclear technology, which are intended for non-control-room personnel of NPP and participants from other organizations, were conducted.

There were 21 radiological protection training courses for the medical, industrial and research use of radioactive sources. Among these, there was a course for security workers during the transport of nuclear materials, and a course for Reactor Centre Podgorica security staff.

We have conducted 4 international courses, 3 in collaboration with the International Atomic Energy Agency Head: (IAEA), and a radiochemistry course that was financed by the EU for the participants from accession countries and **Prof. Igor Jenčič** the lecturers were researchers from the Environmental Sciences Division (0-2).



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 188 groups or 7195 visitors this year. Since 1993 our information centre has been visited by a total of 134,109 pupils,

teachers and other visitors. We have continued monitoring and analyzing 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 has been set up in Bratislava (Slovakia), Vienna (Austria), Strasbourg (France), Antwerp (Belgium) and Biddinghuizen (Netherlands; "road show").

Due to the generation change in NPP Krško the Nuclear Training Centre has conducted very intensive training in the area of nuclear technologies.



Figure 1: Trainees at the Multi-Functional Simulator of the Krško Nuclear Power Plant



Figure 2: Final exam of the Nuclear Technology Course



Figure 4: Trainees at the practical exercises of reactor physics in the control room of the TRIGA reactor



Figure 3: School children on a tour of the control room of the TRIGA reactor

Table of training activities at Nuclear Training Centre in 2011								
Date	e Title			Weeks	Participant × weeks			
(15.11.2010) - 11.4.	15.11.2010) - 11.4. Nuclear technology, theory			14	252			
5.1.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	7	3	0.2	1.4			
31.1 4.2.	Radiation protection for RP department staff - Refresher course	9	9	1	9			
28.2 2.3.	Radiation protection for industrial and other practices (sealed sources)	17	4	0.6	10.2			
28.2 2.3.	Radiation protection for industrial and other practices (unsealed sources)	3	5	0.6	1.8			
7.3 18.3.	IAEA Group Fellowship Training Programme on Research Reactors	5	11	2	10			
8.3 9.3.	Radiation protection for industrial and other practices (radiography) - Re- fresher Course	5	4	0.4	2			
8.3.	Radiation protection for industrial and other practices (sealed sources) - Re- fresher Course	21	4	0.2	4.2			
8.3.	Radiation protection for industrial and other practices (measurement of road- way density and humidity) - Refresher Course	3	4	0.2	0.6			
10.3.	Training Extension for RP Officers	2	2	0.2	0.4			
3.5 30.5.	Basics of nuclear technology, theory	25	10	4	100			
3.5.	Radiation protection for industrial and other practices	23	4	0.2	4.6			
30.5 24.6.	Basics of nuclear technology, systems		8	4	108			
5.9 30.9.	Basics of nuclear technology, theory	27	10	4	108			
23.9.	Radiation Protection	21	1	0.2	4.2			
26.9 6.10.	Interregional Training Course for Nuclear Newcomers on the Physical Protec- tion of Nuclear Material and Facilities	23	5	2	46			
3.10 28.10.	8.10. Basics of nuclear technology, systems		8	4	92			
10.10 12.10.	12.10. Radiation protection for industrial and other practices (unsealed sources)		5	0.6	3			
10.10 12.10.	Radiation protection for industrial and other practices (sealed sources)	12	4	0.6	7.2			
10.10 12.10.	Radiation protection for industrial and other practices (radiography)	1	4	0.8	0.8			
10.10 28.10.	Radiation protection for medical and veterinary workers - Nuclear medicine workers	2	7	1	2			
18.10.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	4	5	0.2	0.8			
18.10 21.10.	Radiation protection for industrial and other practices (radiography) - Re- fresher Course	3	4	0.4	1.2			
18.10.	Radiation protection for industrial and other practices (measurement of road- way density and humidity) - Refresher Course	1	4	0.2	0.2			
18.10.	Radiation protection for industrial and other practices (sealed sources) - Re- fresher Course	10	4	0.2	2			
20.10.	Training Extension for RP Officers	5	2	0.2	1			
7.11 (30.3.2012)	Nuclear technology, theory	15	21	7	105			
7.11 18.11.	IAEA Group Fellowship Training Programme on Research Reactors	4	11	2	8			

Date	Title	Partici- pants	Lecturers	Weeks	Participant × weeks
21.11 2.12.	Training in radiochemistry measurements for practioners from countries eligible under the JRC Enlargement & Integration policy	5	5	2	10
25.11.	Security officers for transport of nuclear materials - Refresher course	13	6	0.2	2.6
8.12 9.12.	Annual refresher course for Security Officers	13	10	0.4	5.2
TOTAL		352	206	53.6	903.4

### INTERNATIONAL PROJECTS

- 1. Public Information in the Association 6.1.1-FU EURATOM – MHEST
  - 7. FP EURATOM, Slovenian Fusion Association SFA
  - FU07-CT-2007-00065

EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Prof. Igor Jenčič

- 2. Fusion Expo Support Action under EFDA Workprogramme, Task Agreement WP10-PIN FUSEX
  - EURATOM MHEST
  - 7. FP EURATOM, Slovenian Fusion Association SFA
  - FU07-CT-2007-00065

EC; RS, Ministry of Higher Education, Science and Technology, Ljubljana, Slovenia Tomaž Skobe, B. Sc., Melita Lenošek Kavčič, B. Sc., Asst. Prof. Igor Lengar, Asst. Prof. Saša Novak Krmpotič

 Realization of the International Workshop: "Group Fellowship Training Programme on Research Reactors" (IAEERRI11), ICJT, 7.-18.3.2011, 7.-18.11.2011 IAEERRI11

Marta Ferrari, IAEA, Department of Nuclear Energy, Division of Nuclear Fuel Cycle and Waste Technology, Vienna, Austria; TU Wien - Atominstitut, Vienna, Austria Saša Bobič, Melita Lenošek Kavčič, B. Sc.

4. Interregional Training Course for Nuclear Newcomers on the Physical Protection of Nuclear

Material and Facilities, (IAPP11)", ICJT, 26.9.-6.10.2011 IAPP11 IAEA, Vienna, Austria Saša Bobič

 Scientific Visitors Mr. Gavrysh and Mr. Minakov from Ukraine E-mail dtd. 17.8.2011
 IAEA, Vienna, Austria Prof. Igor Jenčič

### NEW CONTRACTS

- 1. Operation of the Nuclear Information Centre in 2011 ARAO Agency for Radwaste Management Prof. Igor Jenčič
- Inplementation of 2011 Training Program Nuclear Power Plant Krško Prof. Igor Jenčič

Tomaž Skobe, B. Sc.

Vesna Slapar, B. Sc.

12. Matejka Južnik, M. Sc.

13. Borut Mavec, B. Sc.

Technical and administrative staff

10. Luka Tavčar, B. Sc.

11. Saša Bobič

 Implementation of Training program "Technology of Nuclear Power Plants - Theory" Gen d. o. o. Prof. Igor Jenčič

### STAFF

#### Researchers

#### 1. Prof. Igor Jenčič, Head

- **Technical officers**
- 2. Jure Hribar, B. Sc.
- Rado Istenič, B. Sc.
   Matiaž Koželi, M. S
- Matjaž Koželj, M. Sc.
   Melita Lenošek Kavčič, B. Sc., left 16.04.11
- Mataša Medved, B. Sc.
- 7. Anže Peršin, B. Sc., left 16.05.11

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#### **Regular** papers

- 1. Radko Istenič, Igor Jenčič, "Public opinion about nuclear energy year 2011 poll", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 7 pp.
- 2. Matjaž Koželj, Bruno Cvikl, "On influence of charge traps on free electron transport on conjugated polymers", In: *Proceedings*, 47th International Conference on Microelectronics, Devices and Materials and the Workshop on Organic Semiconductors, Technologies and Devices, September 28 - September 30, 2011, Ajdovščina, Slovenia, Gvido Bratina, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for

Microelectronics, Electronic Components and Materials, 2011, pp. 157-162, 2011.

 Matjaž Koželj, Radko Istenič, "Radioactivity for everyone or twelve years of radioactivity demonstrations in Milan Čopič nuclear training centre", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 8 pp.

#### B. Sc. Thesis

1. Vesna Slapar, *Viscoelastic properties of bacterial meshes:* undergraduate thesis, Ljubljana, [V. Slapar], 2011.

## RADIATION PROTECTION UNIT

## SVPIS

The SVPIS has been involved in ionizing-radiation measurements and radiation protection since the commissioning of TRIGA MARK II Reactor in 1966. The responsibility of the 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 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 a regulatory control.

The SVPIS is authorized by the Slovenian radiation-protection administration to perform the control in medical, industrial and research institutions dealing with open and sealed sources. In industry and research we are authorized to control X-ray units. Furthermore, we are involved in radioactive waste characterization.

The measurements of dose rates, contamination and gamma spectrometry are performed with an accredited method (EN ISO/IEC 17025).

#### **Personal dosimetry**

The personal doses of 124 workers that regularly, or occasionally, deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters (TLDs). The maximum individual yearly dose was 0.07 mSv. This is only 0.4 % of the regulatory limit for occupational exposure (20 mSv per year) and 7 % of the limit for the general public (1 mSv per year). The collective dose at the JSI, in the year 2011, was 0.34 man mSv.

In this year neutron dosimetry was introduced for a small group of employees working at the reactor and accelerator TANDETRON. All the exposures were below the detection limit.

#### Supervision of the reactor and the laboratories

The controlled area of the Reactor, the Hot Cell Facility and the Department of Environmental Sciences was monitored on a weekly basis. During certain activities the constant presence of a radiation-protection worker was needed (i.e., for the opening of the activated samples or for radioactive-waste management). Measurements of dose rates (Figure 1), surface contamination, contamination of different objects and personal contamination were performed routinely. In most cases, no, or very low, contamination levels were measured in the controlled areas. Gamma spectrometry was used to monitor solid, liquid, aerosol, and gas samples, as well as the radioactive waste.

In 2011 we performed 24 inspections in other JSI laboratories. An independent inspection by an external, authorized institution was performed in the SVPIS laboratory and in two JSI laboratories. There were no deficiencies identified that would be important with respect to radiation protection.

At present, 109 sources of radiation are used, which require regulatory control. In addition, another 368 low-activity sources are also used in different laboratories.

Figure 1: Dose rate measurements at the Hot Cell Facility

#### **Environmental measurements**

Environmental monitoring of the Reactor was performed with the measurements of external radiation levels, the measurements of environmental samples and the effluent measurements (gas discharges from the reactor operation and liquid discharges into the Sava River).

With the 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 the normal, natural background radiation levels were recorded.

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 one micro-Sievert per year. In 2011 the public exposure, due to the activities of the Reactor Center, was insignificant.

#### Service for the 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,



Matjaž Stepišnik, M. Sc.

medical and research institutions. Our group has participated in the evaluation of radiological monitoring of Krško NPP, research reactor TRIGA and the storage for low and intermediate level waste in Brinje.

In the scope of international collaboration our members participated in the IAEA missions as experts in the field of radioecology, radiation protection and emergency preparedness.

### STAFF

Technical officers

- 1. Dr. Tinkara Bučar Technical and administrative staff
- Emira Bašić, B. Sc.
- Ellina Basic, B. Sc.
   Thomas Breznik, B. Sc.
- Bogdan Pucelj, M. Sc.

5. Matjaž Stepišnik, M. Sc., Head

## BIBLIOGRAPHY

#### **REVIEW ARTICLES AND CHAPTERS IN BOOKS**

1. Matjaž Stepišnik, "Sava", In: *Ocena vplivov radioaktivnosti v okolici Nuklearne elektrarne Krško na prebivalstvo*, Matjaž Stepišnik, Benjamin Zorko, Denis Glavič-Cindro, ed., 1. izd., Ljubljana, Institut Jožef Stefan, 2011, pp. 1-18.

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#### Regular paper

1. Thomas Breznik, Marko Gerbec, Borut Smodiš, "Task analysis and risk assessment of the transport of the radioactive material by road in the Republic Slovenia", In: *Proceedings*, 20th International Conference Nuclear Energy for New Europe 2011, September 12-15, 2011, Bovec, Slovenia, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2011, 8 pp., 2011.

## 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. The Center was created as a merger of the CT3 financial sub-unit Communication and Technology Transfer (KTT) and the Technology Transfer Office (U9). Its principal activities are the transfer of the technology and the know-how from the JSI to the industry and education, research work in the field of innovation and innovation management, and implementation of specific technology projects. Since 2010 the TT Group has been operational. The TT Group is a joint technology-transfer office of the Jozef Stefan Institute and the National Institute of Chemistry.

In 2011 the CTT was involved in nine major projects. Within the CIP scheme, we were involved in the Enterprise Europe Network and in Slo-Inno-Boost. Within the 7FP we participated in EnvImpact (Increasing the Impact of the Central-Eastern European Environment Research Results through more Effective Dissemination and Exploitation), through the Interreg project we participated in ActClean (Cleaner Production in Central Europe) and we started Head: the project Alps4EU (Alpine Space Clusters Initiative for EU ). The CTT collaborated, as an external partner, in Dr. Špela Stres the European project Intervalue. We were also involved in the national projects: Scientific Meetings (ARRS), KTT

(Communications and Technology Transfer, MVZT) and PROINCOR TP (Technology Park Lj).

We maintain an online entry point with a set of JSI competencies to communicate with the business partners and the general public, http:// tehnologije.ijs.si. We were twice involved in the establishment of a spin-out company and we sold one license to a Slovenian company. In 2011 we dealt with eight patent applications, and participated in two patent applications abroad.

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 50 companies and the researchers have identified over 50 new development projects with fifteen companies. We helped several research departments in the submission of European projects.

During the JSI Open Doors event, last year called the Week of Open Doors, the Institute was visited by more than 1500 visitors and they learned a lot about the Institute, and the structure and activities of individual laboratories. In addition, we recorded throughout the year 65 other visits (and 1660 visitors) from kindergartens, primary schools, high schools, institutions, as well as individuals from all over Slovenia and abroad, who obtained information about the operations of the largest research institution in Slovenia. We also organised field trips for young researchers in four large Slovenian companies and one abroad.

The colleagues at the CTT participated, as organizers or co-organizers, at nine events, as well as attending conferences, forums and round tables. A total of 25 project 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 4th International Technology Transfer Conference, held from 24 to 25 October, 2011. The conference awarded the prize for the most innovative project. The International Commission of the representatives of venture capital awarded the prize of €10,000 for two innovative ideas, coming from the University of Ljubljana and from the Jožef Stefan Institute.



Figure 1: Commission awarding the prize for innovations is evaluating the presented entrees 4th International Technology Transfer Conference (4. ITTC). Photo: F. Podobnik.

We participated in the establishment of two spinout companies and sold a license to a Slovenian company.



Figure 2: JSI Open Doors Day



Figure 3: Staff of the Center for Technology Transfer and Innovation

We visited more than 50 companies. The researchers from the JSI, together with the industrial researchers, identified over 50 new development projects.

#### During the JSI Week of Open Doors there were more than 1500 visitors to the Institute; an additional 65 visits were organized throughout the year, bringing more than 1660 visitors.

Organization of conferences, congress and meetings

PODIM, Round-table on Bioscience, Maribor, 21 April 2011

3rd Jožef Stefan International Postgraduate School Students Confer-

Workshop for young researchers: a spin-off company, Ljubljana, 4

4th International Technology Transfer Conference, from 24 to 25

Mladi upi 1, Ljubljana, 7 June 2011

ence, Ljubljana, 25 May 2011

March 2011

October, 2011.

Mladi upi 2, Ljubljana, 22 September 2011

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3.

4.

5.

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### INTERNATIONAL PROJECTS

1. 2. 3. 4.	EIC&IRC Services in Support of Business and Innovation EACI-EIC&IRC Slovenia 1 CIP - Competitiveness and Innovation EEN-150335 European Commission, Executive Agency for Competitiveness and Innovation (EACI), CIP Network Project Management Unit, Brussels, Belgium Marjeta Trobec, Spec. for International Affairs Slovenian Innovation Boost SLO-INNO-BOOST CIP - Competitiveness and Innovation EEN/SPA/09/INO/257213 European Commission, Executive Agency for Competitiveness and Innovation (EAIC), CIP Network Project Management Unit, Brussels, Belgium Marjeta Trobec, Spec. for International Affairs Increasing the Impact of Central-Eastern European Environment Research Results through more Effective Dissemination and Exploitation ENVIMPACT 7. FP, 265275 EC; Tudomanyos es Technologiai Alapitvany, Hungarian Science and Technology Foundation, Budapest, Hungary Marjeta Trobec, Spec. for International Affairs Cooperation of Space NCPs as a Means to Optimise Services COSMOS 7. FP, 218813 EC; Dr. Adrien Klein, Deutsches Zentrum für Luft und Raumfahrt e.v., (DLR), Köln, Germany Dr. Špela Stres, Dr. Boris Pukl, Prof. Spomenka Kobe Innovation in Science Education - Turning Kids on to Science KidsINNscience 7. FP, 244265 EC, Nadia Prauhart, Markus Meissner, Austrian Institute of Ecology, Österreichisches Ökoogie-Institut, Vienna, Austria	<ol> <li>7.</li> <li>8.</li> <li>9.</li> <li>10.</li> <li>11.</li> <li>12.</li> </ol>	EURIDICE 7. FP, 216271 EC, Dr. Paolo Paganelli, INSIEL - Informatica per il Sistema degli Enti Locali s.p.a, Trieste, Italy Dr. Špela Stres, Marko Grobelnik, Prof. Dunja Mladenić, Mitja Jermol, M. Sc. Reflecting Knowledge Diversity RENDER 7. FP, 257790 EC; Hartmut Schmeck, Karlsruhe Institute of Technology, Karlsruhe, Germany Dr. Špela Stres, Prof. Dunja Mladenić, Marko Grobelnik, Mitja Jermol, M. Sc. Alps 4 EU Alpine Space Operational Programme Partnership Agreement EC; Benedetto Guiseppe, Rossana Borello, Regione Piemonte, Direzione Attivitä Produttive Directorate of Industry and Productive Activities, Torino, Italy Dr. Špela Stres, Tanja Zdolšek Access to Technology and Know-how in Cleaner Production in Central Europe ACT CLEAN Central Europe Programme EC; Jakob Gross, Horst Pohle, Federal Environment Agency, Dessau-Roßlau, Germany Tanja Zdolšek, Andrej Gyergyek, B. Sc., Asst. Prof. Sonja Lojen, Dr. Andrej Stergaršek Slovenia - RTD Technological Audit 2009/0030 30-CE-0262075/00-96 EC; Dr. Stephan Pascall, Andrei Florea, Information Society and Media Directorate - General, Brussels, Belgium Dr. Špela Stres Knowledge Transfer: Tools and Mechanisms for Supporting Innovation 01-747/1 Zoran Vukčević, Directorate for Development of Small and Medium Sized Enterprises, Podgorica, Montenegro Dr. Špela Stres Making Progress and Economic Enhancement a Reality for SMEs
6.	Dr. Špēla Stres, Tomaž Ogrin, M. Sc. European Inter-Disciplinary Research on Intelligent Cargo for Efficient, Safe and Environment-friendly Logistics		MAPEERW SME Keresztesi János, Hungarian Association of IT Companies - Informatikai Vállalkozások

Szövetsége (IVSZ), Budapest, Hungary Dr. Špela Stres 13. Making Progress and Economic Enhancement a Reality for SMEs MaPEer Contract dtd. 13.7.2010 Viktor Stipta, Interactive Net Design Ltd., Miskolc, Hungary Dr. Špela Stres

### STAFF

#### Researchers

Prof. Borut Likar\*, left 01.02.11
 Dr. Špela Stres, Head

#### Technical officers

3. Robert Blatnik, B. Sc.

4. France Podobnik, B. Sc.

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#### PUBLISHED CONFERENCE PAPERS

#### Regular paper

 Špela Stres, Primož Kunaver, "Slovene innovation system regarding SME, implementation strategies, needs, requirements and feedback to overcome barriers for innovation activities", In: Driving forces of creating global ventures: proceedings of the 31st Conference on Entrepreneurship and Innovation Maribor - PODIM, Maribor, 20th-21st April 2011, Miroslav Rebernik, ed., Barbara Bradač, ed., Matej Rus, ed., Maribor, IRP Institute for Entrepreneurship Research, 2011, pp. 227-236.

### NEW CONTRACTS

- 1. Cooperation on assistance in the development and marketing innovation Dr. Špela Stres
- Project Mladiekoin Metodology for Trainers Development Centre Novo Mesto Ltd. Dr. Špela Stres

5. Dr. Andreja Popit, left 01.12.11

- 6. Marjeta Trobec, B. Sc.
- 7. Tanja Zdolšek, B. Sc.

Note: \* part-time JSI member

#### **RESEARCH MONOGRAPH**

1. Mitja Ruzzier, Boštjan Antončič, Elizabeta Zirnstein, Peter Fatur, Tine Nagy, Luka Sešel, Urška Zelič, Peter Slovša, Špela Stres, *Slovenski raziskovalci na razpotju: analiza in predlog ukrepov za spodbujanje in večjo učinkovitost znanstveno-raziskovalne dejavnosti*, Koper, Založba Univerze na Primorskem, 2011.