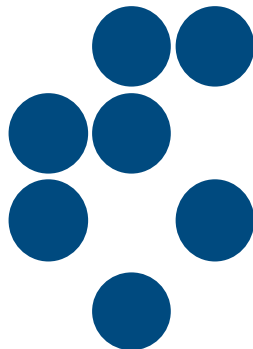


JSI REPORT P-328  
ANNUAL REPORT  
JULY 2015



# Annual Report 2014



Jožef Stefan Institute, Ljubljana, Slovenia

Annual Report 2014

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# INTRODUCTION

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*Prof. Jadran Lenarčič, Director of the Jožef Stefan Institute and Prof. Heinz W. Engl, Rector of University of Vienna, Austria*

*In the early 1990s, when the idea of the Jožef Stefan Gold Emblem came to fruition, we wanted to emphasise the added value of a PhD thesis to society as a whole. Of course, there is nothing remarkable in this, as the Nobel Prizes are awarded to scientists for their contributions to humanity. Therefore, it is hard to understand why such a philosophy is so far from today's measures of scientific excellence, and why we find it so difficult to see beyond a simple reckoning of publications, citations and indices.*

*On the other hand, society now sees science in an increasingly utilitarian light. In other words, what you can't "eat" now, has no value. An Austrian colleague recently told me that in Germany, a technologically successful country, they used to think that a scientist should only investigate what the economy demands. However, very soon, it was the economy that realised that scientists have to work on new ideas and knowledge that might only be useful in 10 or 15 years' time.*

*It seems that in Slovenia the awareness of science, research, creativity and knowledge is on the slide in all spheres of society; this is particularly so in the realm of politics. Therefore, it is not surprising that we can't place scientific research into the general development of society, to the extent required, and which would be eminently possible with only modest efforts and investments. It is also a fact that the investments in research and development have been decreasing since 2009, and this reduction is even greater than in other parts of the public sector. This makes the gap between science and the economy even wider.*

*The scientific and technological success of the Jožef Stefan Institute, which is clearly demonstrated by the content of this annual report, is not the result of the conditions being imposed by the country on science and development, but more in the international breakthroughs of our research groups, mainly through the successful acquisition of European funding, the exchange of researchers, attractive research topics and ambitious goals. For this, the JSI's researchers deserve a great deal of recognition*

*Prof. Jadran Lenarčič  
Director of the Jožef Stefan Institute*

# A BRIEF HISTORY OF THE JOŽEF STEFAN INSTITUTE

1946

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

1949

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

1952

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

1954

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

1956

~ Van de Graaff accelerator, constructed at the institute, started operation

1958

~ Institute reorganised and new fields of activity defined: nuclear physics, solid-state 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,  $XeF_6$ , synthesised at the institute  
~ The first computer for research, ZUSE Z 23, installed

1966

~ Nuclear research reactor TRIGA starts operation

1968

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

1969

~ Institute is renamed as the Jožef Stefan Institute

1970

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

1971

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



*Institute buildings after the opening in 1953*

1972

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

1974

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

1976

~ First Yugoslav 8-bit processor computer DARTA 80

1979

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

1982

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

1983

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



*The Reactor Centre, Podgorica, built in 1966*

1985

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

1987

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



*Nuclear magnetic resonance spectrometer*

1989

- ~ Milan Čopič Nuclear Training Centre established

1990

- ~ The first Slovenian supercomputer, CONVEX, installed at the Jožef Stefan Institute

1992

- ~ 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
- ~ Research institutes in Velenje, ERICo and Valdoltra established by the Institute

1997

- ~ 3.5-MeV electrostatic accelerator, TANDETRON, installed

1999

- ~ Jožef Stefan Institute celebrates its 50<sup>th</sup> anniversary

2003

- ~ 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,  
first Director of the Jožef Stefan Institute*

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 Zavrtnik, 1992–1996

Prof. Vito Turk, 1996–2005

# ORGANISATION OF THE JOŽEF STEFAN INSTITUTE

## BOARD OF GOVERNORS

DIRECTOR

SCIENTIFIC COUNCIL

## RESEARCH DEPARTMENTS

### Physics

**Theoretical Physics (F-1)**

*Prof. Sijetlana Fajfer*

**Low and Medium Energy Physics (F-2)**

*Prof. Primož Pelicon*

**Thin Films and Surfaces (F-3)**

*Asst. Prof. Miha Čekada*

**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. Luka Snoj*

**Experimental Particle Physics (F-9)**

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*Prof. Ingrid Milošev*

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*Prof. Barbara Malič*

**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)**

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**Biotechnology (B-3)**

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**Environmental Sciences (O-2)**

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**Automation, Biocybernetics and Robotics (E-1)**

*Asst. Prof. Aleš Ude*

**Systems and Control (E-2)**

*Dr. Vladimir Jovan*

**Artificial Intelligence Laboratory (E-3)**

*Prof. Dunja Mladenič*

**Open Systems and Networks (E-5)**

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**Communication Systems (E-6)**

*Asst. Prof. Mihael Mohorčič*

**Computer Systems Department (E-7)**

*Prof. Franc Novak, Asst. Prof. Gregor Papa*

**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*

**Networking Infrastructure Centre (NIC)**  
*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)**  
*Milja Jermol, M. Sc.*

**Milan Čopič Nuclear Training Centre (ICJT)**  
*Prof. Igor Jenčič*

**Centre for Electron Microscopy and Microanalysis (CEMM)**  
*Prof. Miran Čeh*

**Centre for Technology Transfer and Innovation (CTT)**  
*Dr. Špela Stres, LL.M.*

**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. Sc.*

**Mass Spectrometry Centre**  
*Dr. Dušan Žigon*

**National Centre for Microstructure and Surface Analysis**  
*Prof. Miran Čeh*

**National Centre for High Resolution NMR Spectroscopy**  
*Prof. Janez Dolinšek*

**Centre for Protein Structure**  
*Prof. Dušan Turk*

**Nanolitography and Nanoscopy**  
*Prof. Dragan Dragoljub Mihailović*

**Centre for Experimental Particle Physics in International Laboratories**  
*Prof. Marko Mikuž*

**Hot Cells Facility**  
*Prof. Borut Smodiš*

**Video-conferencing Centre**  
*Prof. Borka Jerman Blažič*

## ADMINISTRATION, SERVICES AND SUPPORT UNITS

### Administration and Services

**Legal and Personnel (U-2)**  
*Katja Novak, LL. B.*

**Sales and Purchase Department (U-3)**  
*Darko Korbar, M. Sc., MBA*

**Finance and Accounting (U-4)**  
*Regina Gruden, B. Econ.*

**Service for Business Informatics (U-5)**  
*Jože Kašman, B. Sc.*

**Technical Services (TS)**  
*Aleš Cesar, B. Sc.*

### Support Units

**Radiation Protection Unit (SVPIS)**  
*Matjaž Stepišnik, M. Sc.*

**Quality Assurance (QA)**  
*Ljubo Fabjan, M. Sc.*

**Workshops**  
*Franc Setnikar, 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 (SETTCE)

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 Approaches in Chemistry and Biology of Proteins (CIPKeBiP)

Centre of Excellence for Polymer Materials and Technologies (PoliMaT)

CO NOT: Centre of Excellence for Low-Carbon Technologies

EN-FIST Centre of Excellence

Centre of Excellence for Space Sciences and Technologies SPACE-SI



# MANAGEMENT

---

## DIRECTORATE

### Director JSI

Prof. Jadran Lenarčič

### Adviser

Marta Slokan, LL. B.

## BOARD OF GOVERNORS

until April 2014

Prof. Damjan Zazula, *Chair, Ministry of Education, Science and Sport*

Alenka Avberšek, *Ministry of Education, Science and Sport*

Franjo Bobinac, *MBA, Director of Gorenje d. d., Velenje*

Dr. Tomaž Boh, *Ministry of Education, Science and Sport*

Tatjana Fink, *MBA, Director of Trimco d. d., Trebnje*

Prof. Marko Mikuž, *JSI*

Peter Ribarič, *M.Sc., Ministry for Economic Development and Technology*

Prof. Franc Solina, *Ministry of Education, Science and Sport*

Prof. Stanko Strmčnik, *JSI*

since April 2014

Alenka Avberšek, *Chair, Ministry of Education, Science and Sport*

Franjo Bobinac, *MBA, Director of Gorenje, d. d., Velenje*

Dr. Tomaž Boh, *Ministry of Education, Science and Sport*

Prof. Marko Mikuž, *JSI*

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Prof. Jože Pungerčar, *JSI*

Prof. Stanko Strmčnik, *JSI*

Dr. Peter Vrtačnik, *Ministry for Economic Development and Technology*

## SCIENTIFIC COUNCIL

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Prof. Miran Čeh

Prof. Borka Džonova Jerman Blažič

Prof. Milena Horvat

Prof. Spomenka Kobe

Prof. Jadran Lenarčič

Prof. Marko Mikuž

Prof. Ingrid Milošev, *Deputy President*

Asst. Prof. Dunja Mladenić

Prof. Peter Prelovšek

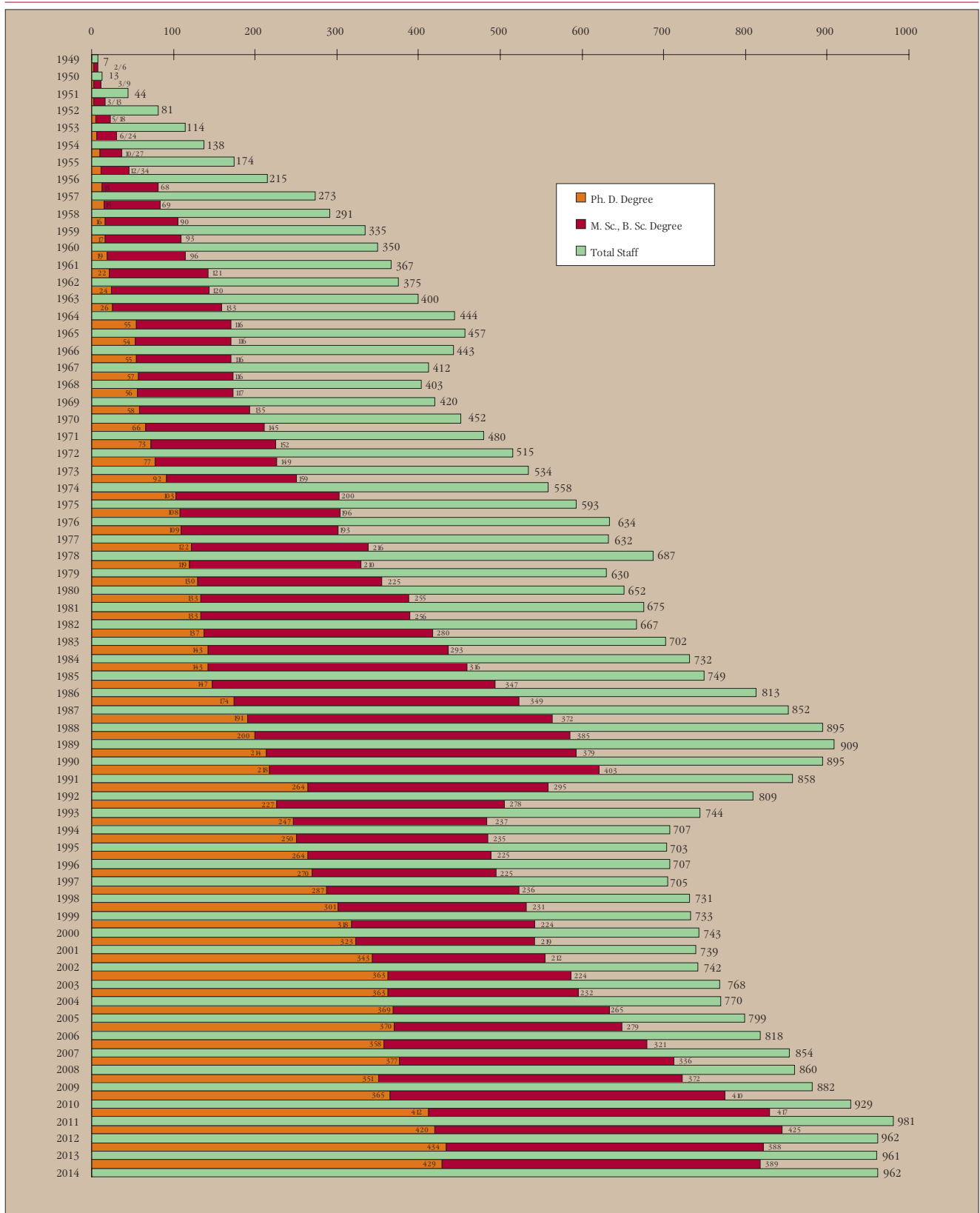
Prof. Žiga Šmit

Prof. Vito Turk

Asst. Prof. Leon Žlajpah, *Deputy President*

# STAFF QUALIFICATIONS

1949-2014



# 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 Frlc, 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
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- Prof. Nobuhiko Katunuma, Tokushima Bunri University, Tokushima, Japan
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- Prof. Herbert W. Roesky, Universität Göttingen, Göttingen, Germany

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- Prof. Findlay E. Russell, The University of Arizona, Tucson, Arizona, USA
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- Prof. Neil W. Tanner<sup>☞</sup>, University of Oxford, Oxford, United Kingdom
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- Prof. Vlado Valković, Zagreb, Croatia
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- Prof. Borut Mavko
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- Prof. Marjan Senegačnik<sup>☞</sup>
- Prof. Saša Svetina
- Prof. Boštjan Žekš
- Prof. Boris Žemva

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- Zdravko Gabrovšek, B. Sc., Slovenia
- Prof. Dušan Hadži, National Institute of Chemistry, Ljubljana, Slovenia
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- Prof. Bogdan Povh, Max-Planck-Institut für Kernphysik, Heidelberg, Germany
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- Milan Slokan<sup>☞</sup>, M. Sc., Ljubljana, Slovenia
- Prof. dr. Petar Strohal, Zagreb, Croatia
- Dr. Novak Zuber, Nuclear Regulatory Commission, Washington D. C., USA
- Prof. Črt Zupančič, Ludwig-Maximilians-Universität, Munich, Germany
- 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

Prof. Robert Huber, *Nobel Prize Winner*, Max-Planck-Institut, Martiensried, Germany

Prof. Karl A. Müller, *Nobel Prize Winner*, Universität Zürich, Zurich, Switzerland

Prof. Ernst Günther Afting, GSF, Neuherberg, Germany

Prof. Akito Arima, Riken, Tokyo, Japan

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Prof. Richard Brook, EPSRC, Swindon, United Kingdom

Prof. Julio Celis, Aarhus University, Aarhus, Denmark

Prof. Brian Clark, Aarhus University, Aarhus, Denmark

Prof. Børge Diderichsen, Novo Nordisk, Bagsvaerd, Denmark

Prof. Jean Etourneau, Institut de Chimie de la Matière Condensée de Bordeaux,  
CNRS, Pessac, France

Prof. Reinosuke Hara, Seiko Instruments, Tokyo, Japan

Prof. Oleg Jardetzky, Stanford University, Stanford, California, USA

Prof. Sergey P. Kapitza, Russian Academy of Sciences, Moscow, Russia

Prof. Karl-Hans Laermann, Bergische Universität, Wuppertal, Germany

Prof. Egon Matijević, Clarkson University, Potsdam, New York, USA

Prof. Federico Mayor, Madrid, Spain

Prof. Dietrich Munz, Universität Karlsruhe, Karlsruhe, Germany

Prof. Günther Petzow, Max-Planck-Institut für Metallforschung, Stuttgart, Germany

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Prof. John Ryan, University of Oxford, Oxford, United Kingdom

Prof. Volker Sörgel, Ruprecht-Karis-Universität, Heidelberg, Germany

Prof. H. Eugene Stanley, Boston University, Boston, Massachusetts, USA

Prof. Thomas Walcher, Universität Mainz, Mainz, Germany

# INTERNATIONAL COOPERATION

Multilateral international cooperation	No. of projects
H2020 (EUROPEAN INSTITUTE OF INNOVATION AND TECHNOLOGY, EXCELLENT SCIENCE, EURATOM, INDUSTRIAL LEADERSHIP, SOCIETAL CHALLENGES, SPREADING EXCELLENCE AND WIDENING PARTICIPATION, SCIENCE WITH AND FOR SOCIETY)	14
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) AND 7. FP - EURATOM	98
ESRR	19
OTHERS (COST, IAEA, EIE, IRMM, ESA, NATO, CIP, CE, SEE, EMRP, WHO, LIFE+, SCOPES, ARTEMIS, EUROSTARS, MNT-ERA.NET IL...)	149
<b>TOTAL</b>	<b>280</b>

Bilateral cooperation	No. of projects
Argentina	3
China	7
Montenegro	2
France	5
Croatia	7
Japan	5
Korea	1

Bilateral cooperation	No. of projects
Russia	5
Serbia	13
Turkey	2
Ukraine	4
USA	21
Others	16
<b>TOTAL</b>	<b>91</b>

## INTERNATIONAL COOPERATION AGREEMENTS

*In 2014, cooperation agreements were signed between the Jožef Stefan Institute and:*

- Babcock & Wilcox Technical Services Y-12, LLC (B&W Y-12), Oak Ridge, TN, USA (F2)
- Institut za medicinska istraživanja i medicinu rada, Zagreb, Croatia (F2)
- Sogang University, School of Natural Sciences, Seoul, Korea (F5)
- Pierre et Marie Curie University, Paris, France (F5)
- Nagoya University, Kobayashi-Maskawa Institute for the Origin of Particles and the Universe, Nagoya, Japan (F9)
- KEK, Tsukuba, Japan (F9)
- VIB vzw, Gent, Belgium (B2)
- CNR Istituto per la Dinamica dei Processi Ambientali, Venezia, Italy (O2)
- Ural Federal University, Ural Center for Shared "Modern Technologies", Ekaterinburg, Russia (K5)
- Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V., München; Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), Dresden, Germany (K6)
- ABB Switzerland Ltd, Corporate Research, Dättwil, Switzerland (K7)
- Aalto University, Department of Materials Science and Engineering, Aalto, Finland (K7, CTT)
- ID Creations oy, Piispanristi, Finland (K7, CTT)
- Stryker Trauma GmbH, Schoenkirchen, Germany (K7, CTT)
- Am Project Design & Consulting SRL, Bucharest, Romania (E2)
- The US National Institute of Standards and Technology, Gaithersburg, Maryland, USA (E3)
- The Universidad de Sonora, Hermosillo, Sonora, Mexico (E6)
- Joanneum Research, Digital Space and Communication Technologies, Graz, Austria (E6)
- Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy (E6)
- A. Menarini Diagnostics S.r.l., Florence, Italy (E7)
- The United Nations Educational, Scientific and Cultural Organization, Paris, France (CT3)
- Meiogenix SAS, Paris, France (B2, CTT)
- IFR - Institute of Food Research, Norwich, Great Britain (E7, CTT)
- Food Angels UK Limited, Suffolk, Great Britain (E7, CTT)
- Asia Center Co., Ltd., Budapest, Hungary (CTT)

# COOPERATION WITH UNIVERSITIES

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7. Prof. Dean Cvetko, University of Ljubljana, Faculty of Mathematics and Physics
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24. Prof. Peter Križan, University of Ljubljana, Faculty of Mathematics and Physics
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27. Prof. Igor Muševič, University of Ljubljana, Faculty of Mathematics and Physics
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30. Prof. Peter Prelovšek, University of Ljubljana, Faculty of Mathematics and Physics
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33. Asst. Prof. Iztok Savnik, University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies

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44. Prof. Slobodan Žumer, University of Ljubljana, Faculty of Mathematics and Physics

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3. Dr. Tomaž Rejec, University of Ljubljana, Faculty of Mathematics and Physics
4. Asst. Prof. Lea Spindler, University of Maribor, Faculty of Mechanical Engineering

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# DELEGATIONS AND VISITORS

Prof. Peter Jenni, University of Freiburg & CERN, Germany & Switzerland,  
14 January 2014

Mr Samo Omerzel, Minister and Mr Danijel Levičar, Director General of Energy  
Directorate, Ministry of the Environment and Spatial Planning of the Republic of  
Slovenia, Ljubljana, 16 January 2014

Ms Alenka Bratušek, M. Sc., Prime Minister of the Republic of Slovenia,  
26 March 2014

*Delegation of Max Planck Society*, Germany, 28 March 2014

Prof. Mordechai Sheves, Vice President for Technology Transfer, Weizmann  
Institute of Science, Israel, 9 May 2014

Prof. Heinz W. Engl, Rector of University of Vienna, Austria, 1 September 2014

Prof. Oliver Smithies, Nobel laureate, University of North Carolina, USA, 10  
September 2014

Marjan Turk, Director General, Information Society Directorate, Ministry of  
Higher Education, Science and Technology of the Republic of Slovenia, Ljubljana,  
10 October 2014

Prof. Toru Iijima, Director, Center for Experimental Studies, KMI Graduate School  
of Science Nagoya University, Japan, 15 October 2014

Prof. Miro Cerar, Prime Minister of the Republic of Slovenia, 27 October 2014

*Chinese delegation*, 18 November 2014

Prof. Christian Thomsen, President, Technische Universität Berlin, Germany,  
25 November 2014

Samo Hribar Milič, M. Sc., President and General Manager, Chamber of Commerce  
and Industry of Slovenia Ljubljana, 10 December 2014

Prof. József Györkös, Director, Slovenian Research Agency, 10 December 2014



*Nobel laureate Prof. Oliver Smithies, University of North Carolina, USA  
during his visit to JSI*

# ART EXHIBITIONS AT THE JSI

Božidar Ted Kramolc, 20 January-20 February

Jendo Štoviček, 24 February-20 March

Metka Krašovec, 24 March-17 April

Nora de Saint Pičman, 23 April-15 May

Peter Škerl, 19 May-19 June

Jasminka Čišić, 23 June-4 September

Jasna Samarin, 8 September-2 October

Milan Rožmarin, 13 October-6 November

Tomaž Gorjup, 10 November-4 December

Irena Gajser, 8 December-15 January 2015



*Metka Krašovec at the opening of her exhibition*

# INSTITUTE COLLOQUIA

15 January: **Gregor Veble**

Pipistrel d.o.o., Ajdovščina and University of Nova Gorica

***Methods for optimization of aerodynamic shapes***

23 January: **Ron M. A. Heeren**

Fundamenteel Onderzoek der Materie - Institute AMOLF, Amsterdam, The Netherlands

***The study of molecular disease profiles with mass spectrometry based molecular imaging approaches***

29 January: **Alessandro Treves**

Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy

***Selforganizing non-Euclidean representations in the brain***

24 February: **Vincenzo Parenti-Castelli**

Università di Bologna, Bologna, Italy

***3D kinematic and kinetostatic models of the knee and the ankle joints***

24 March: **Guido Krömer**

Université Paris Descartes, Hôpital Européen George Pompidou, Institut National de la Santé et de la Recherche Médicale and Institut Gustave Roussy, Paris, France

***Cell death in pathophysiology: inexorable, avoidable or desirable***

25 March: **Janko Kos**

University of Ljubljana and Jožef Stefan Institute

***Ways and sideways of proteolytic enzymes***

26 March: **Djordje Krstić**

***The Einstein family and the visit of Hans Albert Einstein to Jožef Stefan Institute in 1971***

28 March: **Benoît Deveaud-Plédran**

Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

***Vortices and superfluidity in exciton-polariton condensates***

31 March: **Karlheinz Langanke**

GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany

***The universe in the laboratory: FAIR – Facility for Antiproton and Ion Research***

2 April: **Gašper Tkačik**

Institute of Science and Technology Austria, Vienna, Austria

***Critical behavior in networks of real neurons***

16 April: **Maria Leptin**

European Molecular Biology Laboratory, Heidelberg, Germany

***Cell shape and morphogenesis: sub – and supracellular mechanisms***

23 April: **Velimir Bole**

Economic Institute of the Law School, Ljubljana

***Saddle point and economic decline during crisis***

7 May: **Borut Bajc**

Jožef Stefan Institute

***Theories of unification***

28 May: **Nicholas Barton**

Institute of Science and Technology Austria, Vienna, Austria

***Modeling the evolution of flower colour in snapdragons***

4 June: **Kazuki Nakanishi**

Kyoto University, Kyoto, Japan

***Hierarchically porous materials: Preparation and application to separation sciences***

24 June: **Roderick Melnik**

Wilfrid Laurier University, Waterloo, Canada

***Interacting scales and coupled phenomena in nature and models***

1 September: **Heinz W. Engl**

Universität Wien, Vienna, Austria

***The University of Vienna and the RICAM Institute***

10 September: **Oliver Smithies**

University of North Carolina, Chapel Hill, USA

***Where do ideas come from?***

24 September: **Jože Damijan**

University of Ljubljana

***Do we know the recipe to end the crisis?***

10 October: **Miles Berry**

University of Roehampton, London, United Kingdom

***Computer science for all in England***

15 October: **Gabriel Aeppli**

Paul Scherrer Institute, Villingen, Switzerland

***The next life of silicon***

22 October: **Igor L. Pioro**

University of Ontario, Ontario, Canada

***Nuclear power as a basis to future electricity generation***

19 November: **Tomaž Zwitter**

University of Ljubljana

***Interstellar matter***

3 December: **Tomislav Domazet-Lošo**

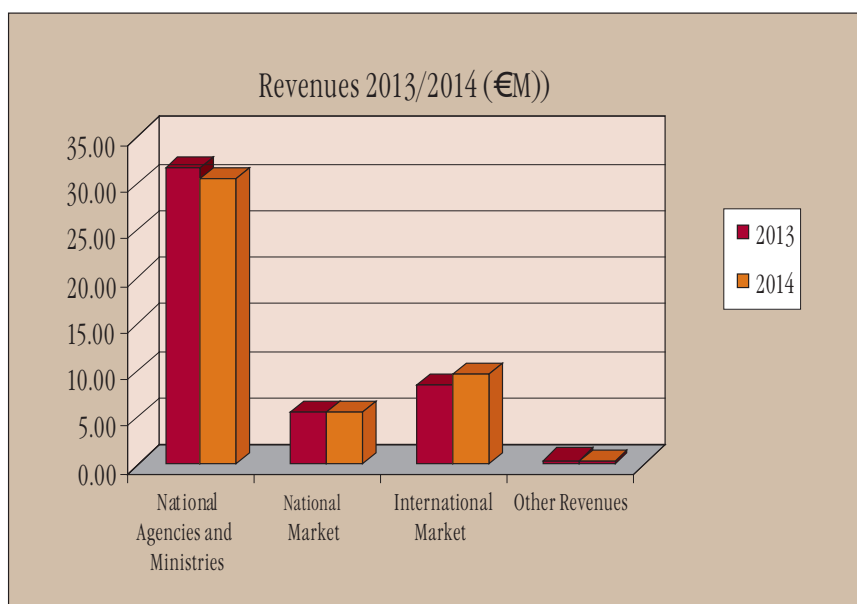
Institut Ruđer Bošković in Hrvatsko katoličko sveučilište, Zagreb, Croatia

***Macroevolution: The roots of good and evil go deep in time***

# FINANCING

## REVENUES JSI (€) AND NUMBER OF PROJECTS

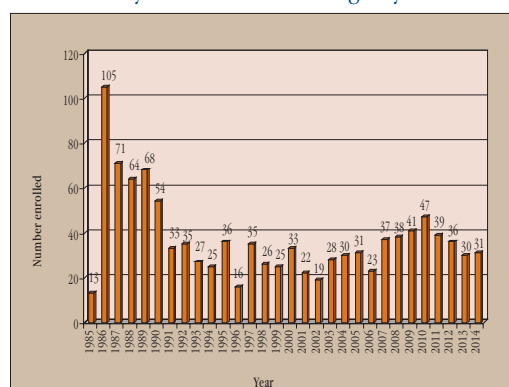
	Contribution		Contribution		Index 2014/2013	No. of Projects in 2014
	2014	2014	2013	2013		
National Agencies and Ministries	30,484,535	66.3 %	31,811,691	68.5 %	95.8	489
National Market	5,487,438	11.9 %	5,598,584	12.0 %	98.0	236
International Market	9,602,339	20.9 %	8,526,897	18.4 %	112.6	330
Other Revenues	402,709	0.9 %	526,217	1.1 %	76.5	
<b>TOTAL</b>	<b>45,977,021</b>	<b>100.0 %</b>	<b>46,463,389</b>	<b>100.0 %</b>	<b>99.0</b>	<b>1055</b>



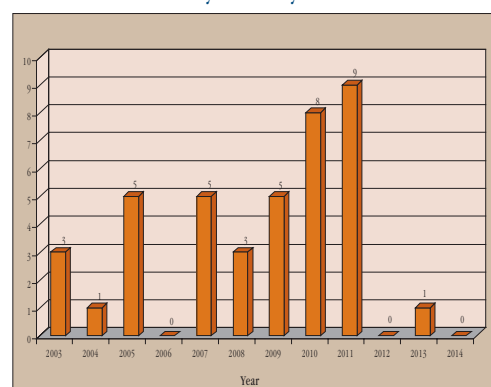
## POSTGRADUATES FINANCED

1985-2014

by Slovenian Research Agency



by Industry





# JSI UNDERGRADUATE SCHOLARSHIPS

1977-2014

Year	FMP		FKKT UNI LJ	FKKT UNI MB	NTF	FDV	FA	BF	FE and FRI	Other UNI LJ	FG and FERI	UNG	IPS	Total
	Physics	Mathematics												
... 1982	115	38	100						50	12				315
1983	10	1	5						9		1			26
1984	11	3	7					1	12		1			35
1985	18	4	6					1	19		1			49
1986	16	8	4						22	2				52
1987	20	8	4						23	2				57
1988	26	7	8					1	27	2				71
1989	26	6	10					1	19	3	1			66
1990	26	5	11					2	25		1			70
1991	23	2	9					2	24	2	1			63
1992	22	3	16					3	17	1				62
1993	21	1	15					3	13	1				54
1994	7	1	8					3	6					25
1995	2		9					3	5					19
1996	2		9					3	5					19
1997	2		12					1	4		1			20
1998	1		6					1	7		1			16
1999	2		7					4	7					20
2000	1		5					3	9					18
2001	3		13					3	10					29
2002	4		20					3	10					37
2003	3		18					2	12	1				36
2004	4		17					1	15	1	2	2		42
2005	3		12			1		2	19		2	1		40
2006	2		12			1		1	17		2	2		37
2007	3		14			1		2	18		2	1		41
2008	2	1	13	3		1		2	15		1	1		39
2009	2	1	17	4		1		5	16		1	2		49
2010	2		11	5	2	1	1	3	10		1	2	5	43
2011	2	1	11	5	4	1	1	4	7		1		6	43
2012	2		10	6	3	1		3	6				5	36
2013	3	2	3	2	1		1		2	2			6	22
2014	14	6	3		2		1		3	2			1	32
TOTAL	400	98	425	25	12	8	4	63	463	31	20	11	23	1583

**FMP** Faculty of Mathematics and Physics, University of Ljubljana  
**FKKT (Uni-Lj)** Faculty of Chemistry and Chemical Technology, University of Ljubljana  
**FKKT (Uni-Mb)** Faculty of Chemistry and Chemical Technology, University of Maribor  
**NTF** Faculty of Natural Sciences and Engineering, University of Ljubljana  
**FDV** Faculty of Social Sciences, University of Ljubljana  
**FA** Faculty of Administration, University of Ljubljana  
**BF** Biotechnical Faculty, University of Ljubljana

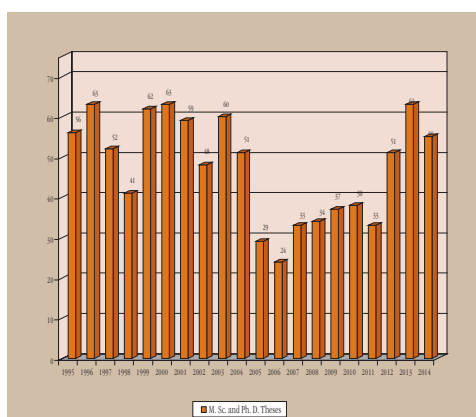
**FE** Faculty of Electrical Engineering, University of Ljubljana  
**FRI** Faculty of Computer and Information Science, University of Ljubljana  
**FG** Faculty of Civil Engineering, University of Maribor  
**FERI** Faculty of Electrical Engineering and Computer Science, University of Maribor  
**UNG** University of Nova Gorica  
**IPS** Jožef Stefan International Postgraduate School  
**Other UNI LJ** Faculty of Pharmacy, Faculty of Mechanical Engineering, Faculty of Economics, Faculty of Medicine, University of Ljubljana

# COMPLETED THESES

UNTIL 2014

Year	Ph. D. Theses	M. Sc. Theses	Total
...1962	15	6	21
1963	7		7
1964	7	2	9
1965	16		16
1966	2		2
1967		8	8
1968	4	8	12
1969	3	6	9
1970	2	12	14
1971	7	6	13
1972	11	24	35
1973	8	14	22
1974	21	10	31
1975	10	20	30
1976	6	31	37
1977	5	16	21
1978	10	20	30
1979	7	11	18
1980	13	10	23
1981	12	15	27
1982	13	18	31
1983	5	10	15
1984	14	17	31
1985	6	14	20
1986	8	15	23
1987	18	21	39
1988	12	26	38

Year	Ph. D. Theses	M. Sc. Theses	Total
1989	15	33	48
1990	16	41	57
1991	22	47	69
1992	19	42	61
1993	28	36	64
1994	27	37	64
1995	34	22	56
1996	38	25	63
1997	29	23	52
1998	21	20	41
1999	33	29	62
2000	36	27	63
2001	31	28	59
2002	29	19	48
2003	41	19	60
2004	31	20	51
2005	22	7	29
2006	22	2	24
2007	26	7	33
2008	29	5	34
2009	30	7	37
2010	33	5	38
2011	31	2	33
2012	47	4	51
2013	56	7	63
2014	51	4	55
<b>TOTAL</b>	<b>1039</b>	<b>858</b>	<b>1897</b>



# PATENTS GRANTED

1. Roman Jerala, Ota Fekonja, Jelka Pohar, Helena Gradišar, Mojca Benčina, Iva Hafner Bratkovič, Robert Bremšak, Špela Miklavič, Urška Jelerčič, Anja Lukan, Tibor Doles, Sabina Božič, Marko Verce, Nika Debeljak, Jožefa Friedrich  
Self-assembled structures composed of single polypeptide comprising at least three coiled-coil forming elements  
EP2488546 (B1), WIPO International Bureau, 31.12.2014.
2. Ita Junkar, Miran Mozetič, Alenka Vesel, Uroš Cvelbar, Metka Krašna, Dragoslav Domanovič  
Method of treatment of biomedical polymeric prosthesis for improvement of their antithrombogenic properties  
AT513072 (B1), Österreichisches Patentamt, 15.2.2014.
3. Mojca Lunder, Matjaž Ravnikar, Borut Štrukelj, Aleš Berlec, Boris Čeh  
Modified food grade microorganism for treatment of inflammatory bowel disease  
US8754198 (B2), United State Patent Office, 17.6.2014.
4. Damjan Kužnar, Matjaž Gams, Domen Marinčič, Marko Lotrič, Klemen Čufar  
Method for intelligent control of refrigeration systems of cooling devices  
SI24163 (A), Slovenian Intellectual Property Office, 28.2.2014.
5. Kristina Žužek Rožman, Paul McGuinness, Marko Soderžnik, Dejan Mir  
Passive magnetic cradle with THWE mechanism of stopping and positioning  
SI24202 (A), Slovenian Intellectual Property Office, 30.4.2014.
6. Matjaž Gams, Tea Tušar, Darko Zadavec, Matej Horvat  
System and method for continuous control and management of tablet manufacturing process  
SI24243 (A), Slovenian Intellectual Property Office, 30.5.2014.
7. Roman Trobec  
Procedure and device for word context window deployment  
SI24263 (A), Slovenian Intellectual Property Office, 30.6.2014.
8. Ljupka Stojčevska, Tomaž Mertelj, Igor Vaskivskiy, Dragan D. Mihailović  
Ultrafast memory by laser quench  
SI24265 (A), Slovenian Intellectual Property Office, 30.6.2014.
9. Matjaž Gams, Hristijan Gjoreski, Mitja Luštrek, Boštjan Kaluža  
Method and system for context-based activity recognition  
SI24356 (A), Slovenian Intellectual Property Office, 28.11.2014.
10. Aleksandra Rashkovska, Roman Trobec  
A procedure and a device for non-invasive control of internal temperature variables in real time between therapy with cooling and heating  
SI24357 (A), Slovenian Intellectual Property Office, 28.11.2014.
11. Marko Šnajder, Nataša Poklar Ulrih, Marko Mihelič, Dušan Turk  
Overproducing recombinant form of pennisine in heterologous expression system  
SI24364 (A), Slovenian Intellectual Property Office, 28.11.2014.

# AWARDS AND APPOINTMENTS

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

### Zois Award and Zois Certificate of Recognition

#### Vito Turk

Presented with the Zois Award for lifetime work

#### Milena Horvat

Presented with the Zois Award for superb achievements in the area of scientific, research, and developmental activities in the field of mercury

### Ambassador of Science of the Republic of Slovenia

Jurij Leskovec



*The winners of Zois Award: Prof. Milena Horvat and Prof. Vito Turk*

## JSI AWARDS AND APPOINTMENTS

### The Jožef Stefan Golden Emblem Prize

*presented to the following for doctoral theses with high impact:*

#### Simon Čopar

Topology and geometry of defects in confined nematics

#### Peter Gregorčič

Non-contact observation of optodynamic phenomena

#### Jure Ačimovič

The effect of Crem gene on circadian expression of lipid metabolites and sterol metabolome in *Mus musculus* mice

### The Jožef Stefan Roll of Honour

*was awarded to companies and institutions for successful scientific and technological cooperation with the Jožef Stefan Institute:*

Danfoss Trata, d.o.o., Ljubljana

Elgoline, d. o. o., Cerknica

Ecological engineering institut, d.o.o., Maribor

*and personal awards to:*

Andrej Božič

Aleksander Zalaznik

Samo Krančan

Miha Bobič

Željko Blažeka

Stane Rožman

## SELECTED OTHER AWARDS TO JSI RESEARCHERS

**Nemanja Aničič**, Best oral presentation at the YUCOMAT 2014 Conference, Herceg Novi, Monte Negro, Materials Research Society of Serbia, awarded talk "The role of morphology and structural characteristics on the solubility of vanadium pentoxide-PLGA composite".

**Ines Bantan, Janez Holc, Danjela Kuščer, Joži Prašnikar, Helena Razpotnik**, Silver acknowledgment for the innovation, Chamber of Commerce and Industry of Slovenia, Zagorje ob Savi, New Cordierite material C410 for the electrotechnics and the procedure of its fabrication

**Simon Čopar**, Glenn Brown Prize, International Liquid Crystal Society

**Boštjan Dolenc** was awarded with the PCT Technology Network award (Process Control Technology) for his Master's thesis entitled "Diagnostics of distributed and localized bearing faults"

**Boštjan Dolenc** was awarded for the best Diploma Thesis at Slovenian state competition on maintenance in 2014 at the 24th Slovenian Trade Fair and Conference on Technical Maintenance

**Boštjan Dolenc** was awarded for his original contribution at the 4th International Conference on Condition Monitoring of Machinery in Non-stationary Operations, CMMNO14

**Peter Dušak**, Best paper according to active participants, Ljubljana, Jožef Stefan International Postgraduate School's Student Council, Preparation of Magnetically-Modified *Oenococcus Oeni*

**Andrej Gams, Tadej Petrič**, Best Scientific Paper Award for outstanding performance and lasting contribution, 23rd International Conference on Robotics in Alpe-Adria-Danube Region, Smolenice, Slovaška, 3. - 5. 9. 2014

**Marinka Gams Petrišič, Gregor Muri, Nives Ogrinc**, Excellence in Science 2013: Source identification and sedimentary record of polycyclic aromatic hydrocarbons in Lake Bled (NW Slovenia) using stable carbon isotopes", ARRS

**Ana Gantar, Rok Kocen, Saša Novak**, "Nanoparticulate bioactive glass-reinforced gellan-gum hydrogels for bone tissue engineering", Best oral presentation at the 22st Conference on Materials and Technology, Portorož, Slovenia, 20–22 October 2014

**Hristijan Gjoreski**, Award for presenting scientific achievements with scientific quality and practical usage, Ljubljana, 6th Jožef Stefan International Postgraduate School Students' Conference, Recognizing human activities and detecting falls in real-time.

**Hristijan Gjoreski, Rok Piltaver**, ECCAI Travel Award 2014, Prague, Czech Republic, European Coordinating Committee for Artificial Intelligence (ECCAI), Multi-objective learning of hybrid classifiers.

**Anton Gradišek**, Fulbright scholarship for work in the ZDA, United States Department of State Bureau of Educational and Cultural Affairs.



*The winners of the Jožef Stefan Golden Emblem Prize: Dr. Simon Čopar, Dr. Peter Gregorčič and Ddr. Jure Aćimović*

**Peter Gselman**, Young researcher award, best oral presentation, Dubrovnik, Croatia, International conference on thin films, "Influence of sulphide and oxide inclusions in steel on growth of TiAlN/CrN nanolayered PVD hard coating"

**Milena Horvat**, Green Week 2014, EU Life+, EU project Democophes; ("Green Week 2014, Best LIFE Environment & Information and Communication projects Award" ), Brussels, Belgium, 4 June 2014

**Jitka Hreščak**, Acknowledgement for the presentation of the research achievements from the view of science quality and their usefulness: Ljubljana, Jožef Stefan International Postgraduate School, The role of different niobium pentoxide precursors in the solid-state synthesis of potassium sodium niobate

**Janez Kokošar, Dušan Kordiš**, Award of the Slovenian Research Agency for an exceptional scientific achievement in 2013 in Slovenia in the field of Biochemistry and Molecular Biology, Genesis and regulatory wiring of retroelement-derived domesticated genes

**Gregor Kosec**, Emerald's awards for excellence: Engineering Outstanding Doctoral Research, Emerald's awards for excellence: Outstanding paper. Second International Conference on Computational Methods for Thermal Problems (ThermaComp 2011), Dalian, China, Solution of a low Prandtl number natural convection benchmark by a local meshless method. V: LI, X. (ur.), September 5-7, 2011, (International Journal of Numerical Methods for Heat & Fluid Flow, ISSN 0961-5539, vol. 23, no. 1). Bradford: Emerald, 2013, vol. 23, no. 1, pp. 189-204.

**Martina Lorenzetti, Thomas Luxbacher, Spomenka Kobe, Saša Novak**, "Zeta Potential: A Useful Tool to Interpret the Hydrothermally Treated Titanium Behaviour

as Biomaterial", Best oral presentation at the ESB2014 (European Society of Biomaterials) Conference, Liverpool, United Kingdom, 3 September 2014

**Tara Nanut**, Honorary document for the students with the best study performance, University of Ljubljana, Ljubljana, Slovenia.

**Miha Nemevšek**, "Apple of quality" 2014, Ljubljana. National recognition is awarded by the Ministry of education, science and sports and the National institute for mobility and european educational and training programmes. The prize was awarded under the Leonardo da Vinci mobility grants for the project of education and collaboration at a foreign institute

**Rok Prebil**, Pregl Award for Outstanding Doctoral Thesis in Chemistry and Related Sciences, Ljubljana, Slovenia, 2014

**Gregor Primc**, 1st award for innovation "Laser Fiber Optic Catalytic sensor". The award was given at 7th International Technology Transfer Conference.

**Igor Shlyapnikov, Evgeny Goreshnik and Zoran Mazej** received recognition from Research Agency of the Republic of Slovenia for outstanding achievement in 2013 in the field of chemistry (Structural architecture of ternary titanium (IV) fluorides) as part of "Excellent in Science 2013".

**Igor Shlyapnikov**, award of the International Postgraduate School Jožef Stefan for exceptional achievements in the year 2014.

**Borut Sluban**, Recognition for outstanding scientific achievement in 2013 by the ARRS as part of the 9th Slovenian Innovation Forum, 13. 11. 2014, "NoiseRank method for detecting anomalies in the data".

**Marko Štrok, Borut Smodiš**, Excellence in Science 2013: Soil-to-plant transfer factors for natural radionuclides in grass in the vicinity of a former uranium mine., Research Agency of the Republic of Slovenia, Ljubljana

**Nejc Trdin**, Best Doctoral Consortium Contribution at the Conference 17th IFIP WG 8.3 DSS 2014, Paris, France, New Generation Platform for Multi-Criteria Decision Making with Method DEX.

**Nejc Trdin**, Inetrnational Postgraduate School's Recognition, Applicant: Dean and President of Jožef Stefan International Postgraduate School

**Roman Trobec** (group leader), "Hekovnik award for "Mobilni EKG" in the frame of the programme start:Something, 21 November 2014."

**Boris Turk**, Lapajne award for outstanding scientific achievements in the field of proteolysis, Ljubljana, Slovenian Biochemical Society

**Vito Turk**, appointment to the Russian Engineering Academy, Vienna, Austria,

**Hana Uršič Nemevšek**, Award at the conference COST MP0904 Action, Bucharest, Romania, Internal Advisory Board of the COST Single-and multiphase ferroics and multiferroics with restricted geometries (SIMUFER), Unusual structural-disorder behavior of Pb(Sc<sub>0.5</sub>Nb<sub>0.5</sub>)O<sub>3</sub>

**Julian Walker**, Excellence Award for the Best Oral Presentation of young scientist, Ekaterinburg, Russian Federation, Organizational Board of the Joint International Conference Piezoresponse Force Microscopy and Nanoscale Phenomena in Polar Materials, Electrical, electromechanical properties and domain structure of Sm-modified-BiFeO<sub>3</sub> ceramics prepared by mechanochemical activation

**Slobodan Žumer**, Honored member of the International Liquid Crystal Society, International Liquid Crystal Society

# REVIEW OF PUBLICATIONS

FOR 2014

Department	Original Articles*	Books	Patent Appl. and Grants	Theses
Department of Theoretical Physics (F-1)	105	4	1	4
Department of Low and Medium Energy Physics (F-2)	68		3	2
Department of Thin Films and Surfaces (F-3)	20			1
Department of Surface Engineering and Optoelectronics (F-4)	73	1	9	2
Department of Solid State Physics (F-5)	111	5	3	5
Department for Complex Matter (F-7)	43	2	3	1
Department of Reactor Physics (F-8)	80			1
Department of Experimental Particle Physics (F-9)	123			2
Department of Inorganic Chemistry and Technology (K-1)	14		1	2
Department of Physical and Organic Chemistry (K-3)	29		1	2
Electronic Ceramics Department (K-5)	65		3	5
Engineering Ceramics Department (K-6)	5			
Department for Nanostructured Materials (K-7)	47		2	6
Department for Synthesis of Materials (K-8)	24			
Department for Advanced Materials (K-9)	31		2	3
Department of Biochemistry, Molecular and Structural Biology (B-1)	36		1	4
Department of Molecular and Biomedical sciences (B-2)	18	1		1
Department of Biotechnology (B-3)	42		4	1
Department of Environmental Sciences (O-2)	104	1	1	4
Department of Automation, Biocybernetics and Robotics (E-1)	51			1
Department of Systems and Control (E-2)	36			2
Artificial Intelligence Laboratory (E-3)	23		1	
Laboratory for Open Systems and Networks (E-5)	12	1		1
Department of Communication Systems (E-6)	41		2	
Computer Systems Department (E-7)	15		1	
Department of Knowledge Technologies (E-8)	56			3
Department of Intelligent Systems (E-9)	58		4	2
Department of Reactor Engineering (R-4)	50	1	1	
Reactor Infrastructure Centre (RIC)	10			
Networking Infrastructure Centre (NIC)	1			
Energy Efficiency Centre (EEC)	17			
Centre for Knowledge Transfer in Information Technologies (CT-3)	3			
Milan Čopič Nuclear Training Centre (ICJT)	2			
Radiation Protection Unit (SVPIS)	3			
Centre for Technology Transfer and Innovation (CTT)	2			
<b>Jožef Stefan Institute</b>	<b>1296</b>	<b>14</b>	<b>42</b>	<b>55</b>

\* 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

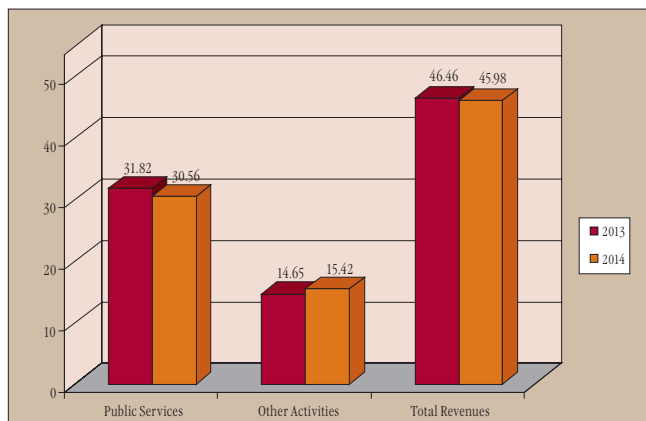
1. Energy Agency, Maribor
2. Bioiks, d. o. o., Ljubljana
3. Central Technological Library at the University of Ljubljana, Ljubljana
4. Danfoss Trata, d. o. o., Ljubljana-Šentvid
5. Ektimo, d. o. o., Medvode
6. Elektro Maribor, d. d., Maribor
7. Energetika Ljubljana, d. o. o., Ljubljana
8. Gen Energija, d. o. o., Krško
9. Golea, Nova Gorica
10. Hermes Analitica, d. o. o., Ljubljana
11. Ecological engineering institut, d. o. o., Maribor
12. Istrabenz Plini, d. o. o., Koper
13. Keko - Oprema, d. o. o., Žužemberk
14. Keko - Varicon, d. o. o., Žužemberk
15. Agricultural Institute of Slovenia, Ljubljana
16. Knauf Insulation, d. o. o., Škofja Loka
17. Kolektor Group, d. o. o., Idrija
18. Krka, tovarna zdravil, d. d., Novo mesto
19. Lek, d. d., Ljubljana
20. City of Ljubljana, Ljubljana
21. Ministry of Finance of the Republic of Slovenia, Ljubljana
22. Ministry of Infrastructure of the Republic of Slovenia, Ljubljana
23. Ministry of Education, Science and Sport of the Republic of Slovenia, Ljubljana
24. Ministry of the Interior of the Republic of Slovenia, Ljubljana
25. Ministry of the Environment and Spatial Planning of the Republic of Slovenia, Ljubljana
26. Slovenian Radiation Protection Administration, Ljubljana
27. Chemicals Office of the Republic of Slovenia, Ljubljana
28. National Institute of Biology, Ljubljana
29. National Laboratory of Health, Environment and Food, Ljubljana
30. Krško Nuclear Power Plant, d. o. o., Krško
31. Institute of Oncology, Ljubljana
32. Plinovodi, d. o. o., Ljubljana
33. RCE - Research Centre Energy, d. o. o., Velenje
34. S2P, science to practice, d. o. o., Ljubljana
35. Splošna bolnišnica Novo mesto, Novo mesto
36. Statistical Office of the Republic of Slovenia, Ljubljana
37. Brestanica Thermal Power Plant, d. o. o., Brestanica
38. Zel-En, Razvojni center energetike, d. o. o., Krško



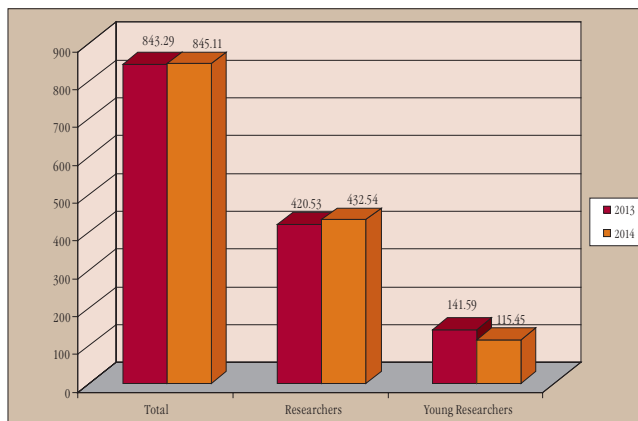
# INSTITUTE IN NUMBERS

2013-2014

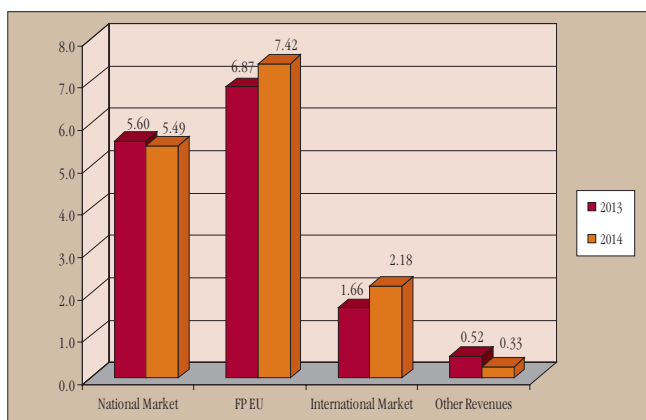
COMPARISON OF REVENUES (€M)



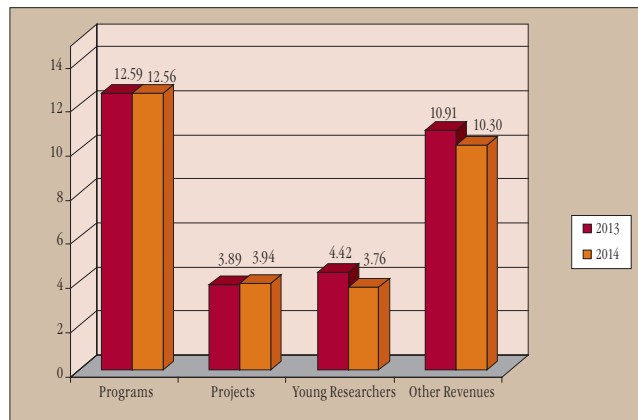
EMPLOYEES (FTE)



REVENUES FROM OTHER ACTIVITIES (€M)



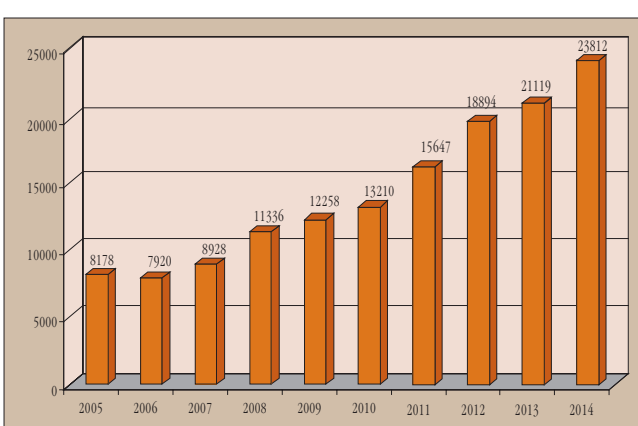
REVENUES FROM PUBLIC SERVICES (€M)



NUMBER OF PUBLICATIONS  
IN THE WEB OF SCIENCE



NUMBER OF CITATIONS  
IN THE WEB OF SCIENCE





# RESEARCH DEPARTMENTS

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# DEPARTMENT OF THEORETICAL PHYSICS

F-1

*The group of Theoretical Physics Of Nuclei, Particles and Fields has investigated the structure of hadrons, the effective theories of weak and electromagnetic mesonic decays, the unified theory of elementary interactions, the relativistic theory of membranes and precise calculations of the properties of three-body systems in atomic physics.*

Positive parity  $D_s$  mesons were expected above the  $D^*K$  threshold, but were experimentally found below them. We performed the first lattice QCD simulation that takes into account the effect of the nearby threshold. The effect lowers their masses and renders them in agreement with experiment. For this purpose we simulated the  $D^*K$  scattering and searched for the pole of the scattering matrix. We performed the first lattice QCD study of the light axial resonances  $a_1$  and  $b_1$  that takes into account their strong decays.

We studied the possibility of detecting New Physics (NP) phenomena at the LHC through a new search strategy looking at the monotop (top plus missing energy) signature, which is common to a variety of NP models. We focus on the leptonic top decay mode and study the discovery or exclusion reach of the 2012 LHC data for three example models.

We studied the LHC phenomenology of flavour-changing Yukawa couplings between the top quark, the Higgs boson, and either an up or charm quark. Such  $tuh$  or  $tch$  couplings arise for instance in models in which the Higgs sector is extended by the existence of additional Higgs bosons or by higher dimensional operators. We emphasized the importance of the anomalous single top plus Higgs production in these scenarios, in addition to the more widely studied  $t \rightarrow hj$  decays. We then investigated the sensitivity of future searches in the multi-lepton channel and in the fully hadronic channel.

We studied the implications of large lepton-quark-leptoquark couplings for direct leptoquark searches at the Large Hadron Collider. We have investigated the implications of enlarging the Standard Model fermion sector by either one light singlet vector-like down-type quark or one light vector-like lepton doublet and we have determined their impact on the mass matrices. We studied new contributions to the neutron electric dipole moment induced by coloured scalars.

We explicitly found a candidate for a realistic renormalizable supersymmetric E6 model. The Higgs sector with 351 and 27 dimensional representations breaks E6 directly to the standard model, while an extra 27 dimensional pair performs the doublet-triplet splitting. We perform the analysis of the vacuum structure, the Yukawa sector, and compute the contributions to proton decay.

We studied the strong CP violation in the minimal Left-Right (LR) symmetric model. When generalized parity is restored, the strong CP phase is computed and bounded by the neutron electric dipole moment. This requires a small spontaneous phase and fixes the flavour of all the interactions, while keeping the quantum corrections under control. Indirect CP violation in the kaon sector then sets a limit on the LR scale. We discussed possible evasions and the case of charge conjugation as LR parity.

A nonparametric, purely numerical regularization of the nonperturbative Quasilinearization Method (QLM) for nonlinear differential equations was developed, applicable to regular and very singular potentials. Exponentially singular potentials showed a uniform quadratic convergence of the energy to a nearly machine precision of 30 digits in just 4 to 8 QLM iterations.

## Some outstanding publications in the past year

1. Isidori, G., Kamenik, J.: Shedding light on CP violation in the Charm system via DV decays. Physical review letters, ISSN 0031-9007. [Print ed.], 2012, vol. 109, no. 17, 171801-1-171801-5, ilustr., doi: 10.1103/PhysRevLett.109.171801. [COBISS.SI-ID 26206759]



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**Prof. Sijetlana Fajfer**

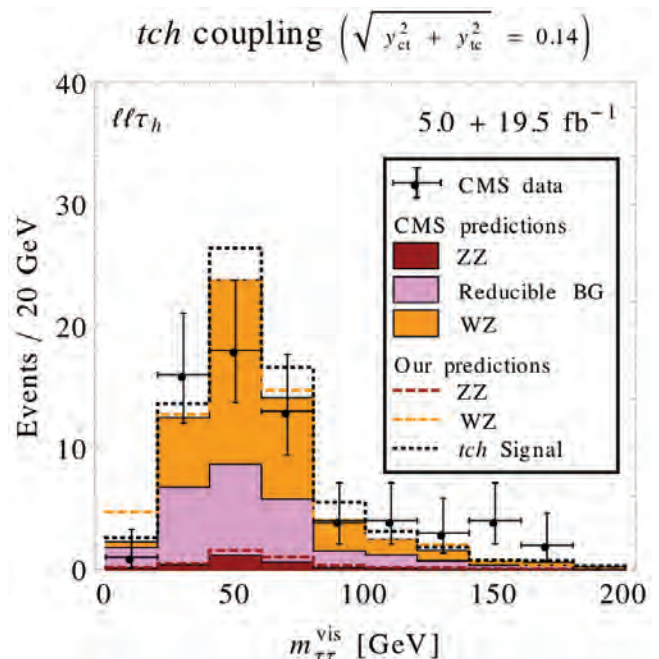


Figure 1: Comparison of flavour-violating  $pp \rightarrow (t \rightarrow Wb) (t \rightarrow hc)$  and  $pp \rightarrow th$  signals to the data from a CMS search for vector boson + Higgs production in the final states with two light leptons and a hadronically decaying tau lepton. We plot the number of events against the invariant mass of the tau jet and the two light leptons. The data points correspond to the CMS measurement in  $5.0 \text{ fb}^{-1}$  of 7 TeV data and  $19.5 \text{ fb}^{-1}$  of 8 TeV data. The measurement can be used to constrain the flavour-violating top-charm-Higgs couplings ( $y_{ct}$  and  $y_{tc}$ ).

*The group of Solid State Theory and Statistical Physics has been investigating the equilibrium and non-equilibrium properties of materials with strongly correlated electrons, nanosystems, as well as the properties of complex networks.*

**We investigated the sensitivity of future LHC searches for top quark flavour-changing Higgs Yukawa couplings in the multi-lepton decay channel and in the fully hadronic channel. We developed the first complete case of a E6 grand unified theory. A study of strong CP violation reveals a strong constraint on the scale of Left-Right symmetry if parity is restored at high energies.**

analysis extended to a realistic charge-transfer model for undoped cuprates. The direct numerical simulations of the recombination have also been compared to the analytical results. Using the density-matrix the time-evolution approach we established that an integrable interacting many-body system with a nonzero current in an initial state does not obey the generalized Gibbs-ensemble hypothesis. We also studied heat and electric current as well the Pelter effects in a one-dimensional model of driven correlated electrons.

**We proved that single qubit gates can be realized and that the two-qubit fully entangled gate can be achieved in two neighbouring dots, interacting via the Coulomb interaction.**

In the theory of non-equilibrium properties of correlated electrons we continued our research on various prototype models with the emphasis on the numerical simulation of undoped and weakly doped Mott insulators. We studied the relaxation mechanism of a highly excited charge carrier in the antiferromagnetic background. We have shown that the relaxation consists of two distinct stages. In the initial, ultrafast stage the relaxation is based on the generation of local string states in the close proximity of the carrier. In the subsequent, much slower, stage, local antiferromagnetic excitations are carried away by magnons. The influence of additional coupling to the phonons has also been investigated. The recombination of carriers photoexcited in a Mott insulator has been further studied and the single-band theory in the low-frequency range and the universal non-Fermi liquid signatures in the higher-frequency range. We found quantum oscillations in CaRuO<sub>3</sub> as well deviations from the Drude form. In the field of the impurity quantum sub-gap state two major projects have been completed: i) a study of the effects of an additional normal-state tunnel contact and of the magnetic field on a quantum dot, coupled to a superconductor, ii) a systematic study of the spectra of impurity states in the system of serial double quantum dot. We showed that the impurities modelled by random exchange interactions in the quantum spin chain lead to a reduced ordered magnetic moment with a large local spread in the ordered phase and reduced transition temperature. In collaboration with the calorimetry group we have considered the models for the electro-caloric effect in PbZrO<sub>3</sub> and for the freezing of the polarization in dipolar glasses and relaxor ferroelectrics.

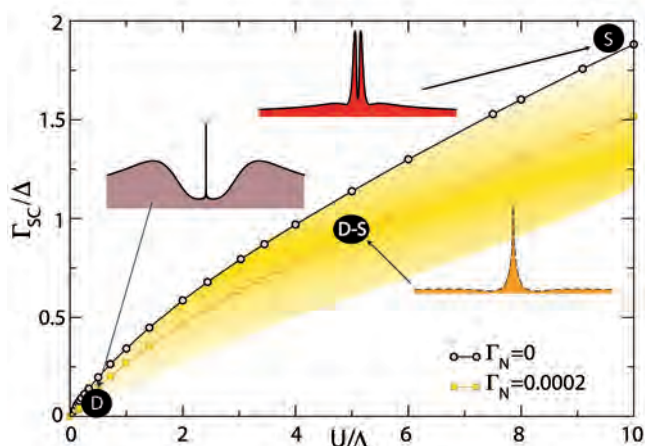


Figure 2: Phase diagram of the quantum dot with Coulomb interaction  $U$ , coupled to a superconductor and to a normal-state tunnelling probe. The insets show the characteristic spectra in the different regimes.

Within the theory of nanoscale systems we studied qubit gates as a coherent evolution of a few electron states in quantum dots in the presence of the Rashba coupling. We proved that single qubit gates can be realized and that the two-qubit fully entangled gate can be achieved in two neighbouring dots, interacting via the Coulomb interaction. We implemented a numerical method to calculate the transport properties of time-dependent systems consisting of a central nanoscopic region attached to a number of translationally invariant electrodes.

In the research of the statistical physics of complex systems and networks we analysed the empirical data from the world-wide-web network and theoretically modelled it. We also simulated nano-systems using mathematical graphs of the nano-network.

Within the CYBEREMOTIONS project we studied the agent-based modelling approach, whereby the appearance of collective states is examined as well as their response to random and coherent perturbations.

### Some outstanding publications in the past three years

1. Čadež, T., Jefferson, J. H., Ramšak, A.: Exact nonadiabatic holonomic transformations of spin-orbit qubits, Phys. Rev. Lett. 112, 150402 (2014)
2. Mierzejewski, M., Prelovšek, P., Prosen, T.: Breakdown of the generalized Gibbs ensemble for current-generating quenches, Phys. Rev. Lett. 113, 020602 (2014)

***The group for Theoretical Biophysics and Soft Matter Physics investigated polyelectrolytes, liquid crystals, colloids, and phospholipid and biological membranes.***

We studied the effects of disorder on confined Coulomb fluids and liquid crystals. A field theoretical description of the Kirkwood–Schumaker was analysed for one- and three-dimensional systems. We described the effects of the ionic solution bath on the charge of the viral capsids and on the electrostatic interactions involved in packing of the RNA genome into the capsid. The Lifshitz theory of van der Waals interactions was used to assess their strength in various molecular systems and interaction geometries. We studied the evolution of the physical compactness of the genome of icosahedral RNA viruses. Using molecular dynamics modelling we quantified the nature of the hydration and hydrophobic forces acting between various biological membranes and surfaces in water environments.

Also investigated was the short-range order in the liquid phase of dendrimer macromolecules, finding that their average shape is somewhat elongated and that neighbouring dendrimers are preferentially perpendicular to each other. We studied knotted or charged polymers under tension and the organization of nanoparticles within grafted polymer layers, showing that mechanical pressure can be an efficient tool to drive the pattern formation and control the morphology of the emerging structures. Our findings may represent a basis for diverse applications in the area of miniature sensing, structured thin films or photovoltaics. We analysed a simple model of interparticle interaction which captures the behaviour of core-shell nanocolloids, and we discovered several types of quasicrystalline phases with 10-, 12-, and 18-fold symmetry.

We theoretically showed that flexoelectricity is the driving mechanism for the formation of several modulated nematic phases observed in materials formed by chiral dimers. Also studied was the effect of the bias electric field on the dielectric response of thin ferroelectric smectic cells. We determined the structure of three-dimensional phases made of rod-like molecules and described the occurrence of huge bend elastic constant in compounds with an azo-linkage. We finalized some of our theoretical studies of interactions to more distant layers in a smectic liquid crystal. Also explored was the transfer of new research results to liquid-crystal education.

We studied the evolution of enzymes and we demonstrated that the principle of maximal production of reaction entropy can also be used to model the more complex enzyme reactions. We continued to investigate the metabolism of arachidonic acid and we extended the existing model by taking into account several new metabolites prostaglandins.

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**Coupling between electrostatic interactions and various types of thermal and structural disorder can lead to novel antifragile material behaviour.**

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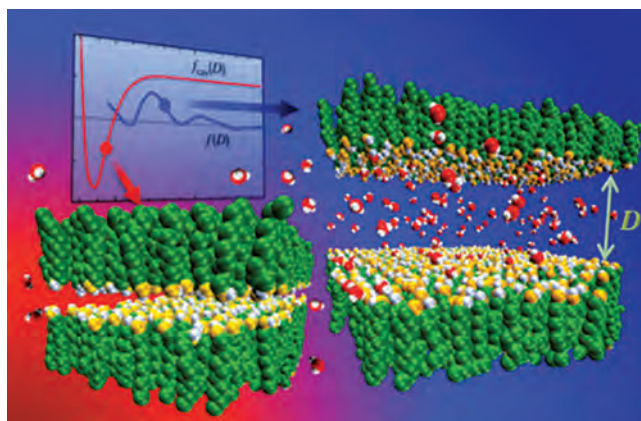


Figure 3: Numerical simulations show that the nature of interactions between surfaces in water is governed by a subtle balance of hydrogen bonds.

### Some outstanding publications in the past year

1. Doter, T., Oshiro, T., Zihel, P.: Mosaic Two-Lengthscale Quasicrystals. *Nature*, ISSN 0028-0836, 506 (2014) 7487, 208–211
2. Curk, T., Martinez-Veracoechea, F. J., Frenkel, D., Dobnikar, J.: Nanoparticle Organization in Sandwiched Polymer Brushes. *Nano Letters*, ISSN 1530-6984, 4 (2014) 5, 2617–2622

### Patent granted

1. Roman Jerala, Ota Fekonja, Jelka Pohar, Helena Gradišar, Mojca Benčina, Iva Hafner Bratkovič, Robert Bremšak, Špela Miklavič, Urška Jelerčič, Anja Lukan, Tibor Doles, Sabina Božič, Marko Verce, Nika Debeljak, Jožefa Friedrich, Self-assembled structures composed of single polypeptide comprising at least three coiled-coil forming elements, EP2488546 (B1), WIPO International Bureau, 31.12.2014.

### Awards and appointments

1. Dr. Miha Nemevšek: ‘Apple of quality’ 2014, Ljubljana. National recognition is awarded by the Ministry of education, science and sports and the National institute for mobility and european educational and training programmes. The prize was awarded under the Leonardo da Vinci mobility grants for the project of education and collaboration at a foreign institute.

### Organization of conferences, congresses and meetings

1. SUMMERSOLSTICE 2014, International Conference on Discrete Models of Complex Systems, Ljubljana, 22.-25. 6. 2014
2. Dynamics of Quantum Many-Body Systems far from Equilibrium, Krvavec, 14.-17. 12. 2014



## INTERNATIONAL PROJECTS

1. COST TD1210; Analysing the Dynamics of Information and Knowledge Landscapes  
Prof. Bosiljka Tadić  
COST Office
2. Aspects of the AdS-CFT Correspondence in Particle Physics and Cosmology  
Prof. Borut Bajc  
Slovenian Research Agency
3. Relaxation Dynamics of Correlated Electron Systems  
Prof. Janez Bonča  
Slovenian Research Agency
4. Higgs Boson at the Junction of Flavor Physics and Dark Matter  
Asst. Prof. Jernej Fesl Kamenik  
Slovenian Research Agency
2. Biophysics of Polymers, Membranes, Gels, Colloids and Cells  
Prof. Rudolf Podgornik

## R & D GRANTS AND CONTRACTS

1. Non-equilibrium Dynamics of Interacting Electron Systems  
Prof. Peter Prelovšek
2. Integrability and Ergodic Theory of Non-equilibrium Quantum Many-body Systems  
Dr. Jernej Mravlje
3. Theoretical Aspects and Empirical Analysis of Labour Market Impact of Flexicurity  
Dr. Jernej Mravlje
4. International Conference: SUMMERSOLSTICE 2014 International Conference on Discrete Models of Complex Systems, Ljubljana, Slovenia, 22-25 June 2014  
Prof. Bosiljka Tadić

## RESEARCH PROGRAMS

1. Theory of the Condensed Matter and Statistical Physics  
Prof. Janez Bonča

## VISITORS FROM ABROAD

1. Dr. Chu Xiaoyong, ICTP, Trieste, Italy, 5.-9. 1. 2014
2. Dr. Jose Juknevič, SISSA v Triesteu, Italy, 9. 1. 2014
3. Dr. Federico Mescia, Dep. d'Estruttura i Constituents de la Materia (ECM) and Institut de Ciències del Cosmos (ICC), Universitat de Barcelona, Spain, 5.-8. 2. 2014
4. Dr. Christoph Bobeth, Technische Universität München, Germany, 16.-18. 2. 2014
5. Dr. Stephane Lavignac, Saclay Paris, France, 18.-22. 2. 2014
6. Prof. Dr. Guillermo Silva, IFLP-Departamento de Física, UNLP, La Plata, Argentina, 20. 2. 2014
7. Dr. Oscar Cata, Technische Universität München, München, Germany, 24.-26. 2. 2014
8. Dr. Claudia Hagedorn, Univerza v Padovi in SISSA, Trieste, Italy, 26.-28. 2. 2014
9. Dr. Ryan Requist, Condensed Matter Theory and Simulation, Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy, 3. 3. 2014
10. Prof. Dr. Marcin Mierzejewski, University of Katowice, Katowice, Poland, 10.-22. 3., 7.-12. 4. and 30. 6.-12. 7. 2014
11. Dr. David Civelli, University of Katowice, Katowice, Poland, 10.-22. 3. 2014
12. Dr. Luca Celardo, Interdisciplinary Laboratories for Advanced Materials Physics (i-LAMP) Università Cattolica del Sacro Cuore, Brescia, Italy, 17.-19. 3. 2014
13. Dr. Diptimoy Ghosh, Sapienza - Università di Roma, Rim, Italy, 19.-21. 3. in 21.-23. 7. 2014
14. Dr. Armando Amaricci, SISSA, Trieste, Italy, 1. 4. 2014
15. Prof. Dr. Ilja Doršner, Sarajevo University, Institute of Natural Sciences and Mathematicse, Sarajevo, BIH, 6.-12. 4., 20.-26. 4., 25. 5.-25. 6., 22. 7.-16. 8., 24. 8.-26. 8., 23. 12. 2014-6. 1. 2015
16. Dr. Yigal Meir, Ben Gurion University, Department of Physics, Beer Sheva, Israel, 20.-22. 4. 2014
17. Dr. Jacek Herbrych, University of Heraklion, Heraklion, Greece, 22.-29. 4. 2014
18. Prof. Dr. Guido Martinelli, SISSA-ISAS, Trieste in INFN Sezione di Roma, Italy, 12. 5. 2014
19. Prof. Dr. Bing-Su Lu, Shanghai Jiao Tong University, Shanghai, China, 26. 5.-28. 5. 2014
20. Prof. Dr. Darko Tanasković, Institut za Fiziko, Beograd, Serbia, 8.-12. 6. 2014
21. Mag. Willem-Victor van Gerven Oei, Institut for Physics, Beograd, Serbia, 8.-12. 6. 2014
22. Dr. Enrico Arrigoni, Institute of Theoretical Physics and Computational Physics, Graz University of Technology, Graz, Austria, 18.-20. 6. 2014
23. Dr. Panagiotis Kotetes, Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany, 18.-22. 6. 2014
24. Dr. Dipankar Das, Saha Institute Of Nuclear Physics, Kolkata, India, 28. 6.-13. 7. 2014
25. Dr. Yu Muramatsu, Theoretical Particle Physics Group, Nagoya University, Japan, 29. 6.-2. 7. 2014
26. Prof. Dr. Damir Bečirević, Laboratoire de Physique Theorique d'Orsay, Univ. Paris-Sud, France, 1.-3. 7. in 10.-28.11. 2014
27. Prof. Dr. Adrian Lugo, Departamento de Física and IFLP-CONICET, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, La Plata, Argentina, 7.-14. 7. 2014
28. Dr. Wolfgang Altmannshofer, Perimeter Institute for Theoretical Physics, Waterloo, Canada, 3.-5. 9. 2014
29. Dr. Rafaelo Patesio, Max Planck Institute Mainz, Germany, 4.-9. 9. 2014
30. Prof. Dr. Antonio Šiber, Institut za fiziku, Zagreb, Croatia, 15. 9. do 15. 12. 2014
31. Dr. Takehiro Jimbo, Tohoku University, Sendai, Japon, 1.-30. 10. 2014
32. Dr. Marco Nardecchia, Centre for Particle Physics Phenomenology, CP3-Origins, University of Southern Denmark, Odense, Denmark, 6.-10. 10. 2014
33. Dr. Luca di Luzio, Karlsruhe Institute of Technology, Karlsruhe, Germany, 6.-30. 10. 2014
34. Dr. Ramona Groeber, Karlsruhe Institute of Technology, Karlsruhe, Germany, 15.-24. 10. 2014
35. Prof. Dr. Masayuki Imai, Ochanomizu University, Tokio, Japon, 16.-19. 10. 2014
36. Prof. Dr. Ivica Picek, Naravoslovno-matematički fakultet, Zagreb, Croatia, 24. 9. 2014
37. Miroslav Andjelković, mag., Institut Vinča, Beograd, Serbia, 28. 10.-28. 12. 2014
38. Dr. Sacha Davidson, Institut de Physique Nucleaire de Lyon, Lyon, France, 4.-7. 11. 2014
39. Dr. Mikhail Kiselev, ICTP, Trieste, Italy, 4. 11. 2014
40. Dr. Madanagopalan Padmanath, Institute of Physics, Karl-Franzens-Universität Graz, Graz, Austria, 2.-8. 11. In 16.11.-6. 12. 2014
41. Prof. Dr. Anthony Maggs, Laboratoire de Physico-Chimie Théorique, ESPCI, Paris, France, 9. 11. 2014
42. Prof. Dr. Stuart A. Trugman, Los Alamos National Laboratory, Los Alamos, USA, 13.-19. 12. 2014
43. Prof. Dr. Xenophon Zotos, University of Crete, Heraklion, Greece, 13.-20. 12. 2014
44. Prof. Dr. Adrian Feiguin, Northeastern University, Department of Physics, Boston, USA, 14.-17. 12. 2014
45. Dr. Admir Greljo, Universität Zürich, Physik-Institut, Zürich, Switzerland, 15.-19. 12. 2014

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30. Dr. Matej Kanduč
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32. Dr. Luca Tubiana, left 01. 12. 14
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34. Dr. Lev Vidmar

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39. Jan Kogoj, B. Sc.
40. Matej Krajnc, B. Sc.
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43. Luka Leskovec, B. Sc.

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48. Dr. Vasja Susič

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# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Puja Adhikari, Amy M. Wen, Roger H. French, Vozken Adrian Parsegian, Nicole F. Steinmetz, Rudolf Podgornik, Wai-Yim Ching, "Electronic structure, dielectric response, and surface charge distribution of RGD (1FUUV) peptide", *Scientific reports*, vol. 4, art. no 5605, 7 pp., 2014.
2. Nataša Adžić, Rudolf Podgornik, "Field-theoretic description of charge regulation interaction", *The European physical journal. E, Soft matter*, vol. 37, iss. 6, 12 pp., 2014.
3. Ezequiel Alvarez, Estefania Coluccio Leskow, Jure Drobnak, Jernej Kamenik, "Leptonic monotops at the LHC", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 89, no. 1, pp. 014016-1- 014016-15, 2014.
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26. Mojca Čepič, "Systems with competing interlayer interactions and modulations in one direction: finding their structures", *ChemPhysChem*, vol. 15, no. 7, pp. 1297-1309, 2014.
27. Mojca Čepič, "Teaching liquid crystals - observation inspired curiosity: [invited article]", In: Special issue of the 24th International Liquid Crystal Conference, August 19th - 25th 2012, Mainz, *Liq. cryst.*, vol. 41, no. 3, pp. 452-464, 2014.
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# DEPARTMENT OF LOW AND MEDIUM ENERGY PHYSICS

# F-2

*The Department of Low and Medium Energy Physics is active in research in the field of atomic physics (low-energy physics) and nuclear physics (medium-energy physics). The research work at the department is done in collaboration with distinguished domestic and international research institutions. The research in physics at the department is extending to interdisciplinary research, solving problems in the fields of material research, biology, medicine, pharmacy and archaeology. We invest a lot of efforts in the development of our own research instrumentation, which is frequently used by visiting researchers from abroad. The research at the ion accelerator of the Microanalytical Centre is complemented with a series of experiments at the large research facilities worldwide, including particle accelerators, synchrotrons, free-electron lasers and fusion reactors.*



Head:  
**Prof. Primož Pelicon**

In the A1 Collaboration of the MAMI facility (Mainz, Germany) we have completed the last data-acquisition period of the virtual Compton scattering by measuring the only remaining kinematic setting with  $0.5 \text{ GeV}^2$ . At present we are in possession of all three planned data sets at momentum transfers of 0.1, 0.2 and  $0.5 \text{ GeV}^2$  that will enable us to determine the generalized polarizabilities of the proton. By repeating one kinematic setting of the measurement in the region of the Roper resonance we have obtained additional statistics for the determination of the resonance amplitudes in the neutral-pion electroproduction off protons. We have continued with our measurements of the elastic scattering of electrons on protons, in which the initial-state radiation (ISR) method is used to access the range of momentum transfers otherwise unreachable in a standard spectrometer configuration. The main goal of the experiment is the determination of elastic (electric and magnetic) form factors of the proton at momentum transfers below approximately  $0.01 \text{ GeV}^2$ , thereby opening a way to the determination of the mean value of the proton radius, where the discrepancy between the values extracted from electron scattering and those determined in Lamb-shift measurements in muonic atoms remains unresolved. We have performed another search of “dark photons”, i.e., the hypothetical particle that might couple ordinary and dark matter.

At the Thomas Jefferson National Accelerator Facility (Jefferson Lab) we have performed the first run of the real Compton scattering experiment at high momentum transfers, implying also large values of all the Mandelstam variables  $s$ ,  $t$  and  $u$ . We have also completed the first part of the production running of the elastic magnetic form-factor experiment at high momentum transfers (up to  $18 \text{ GeV}^2$ ). Both experiments mentioned above are the first ones that came on the floor in Hall A after the  $12 \text{ GeV}$ -upgrade of the CEBAF accelerator. We have published the first paper reporting on our studies of proton and deuteron knock-out from  $^3\text{He}$ , as well as a high-impact paper in Nature on our previous studies of parity violation in deep inelastic electron-quark scattering (Wang et al, Nature 2014).

In order to further investigate the electron-screening effect in nuclear reactions, we studied nuclear reactions involving low charge number targets in different metallic environments: Zn, Pd, Pt and Ni. Hydrogen was implanted into the targets using our ion gun. We have studied the  $^1\text{H}(^7\text{Li},\alpha)^4\text{He}$  reaction in inverse kinematics. Large electron screening of a few keV was observed in all targets. In a continuation of our experimental campaign we further investigated the  $^1\text{H}(^7\text{Li},\alpha)^4\text{He}$  reaction in W, Pd and C environments. We implanted hydrogen into a structurally damaged W target using an ion gun. Hydrogen was absorbed into the damaged Pd foil from the gas phase. In addition, we also focused on studies of electron screening in the  $^1\text{H}(^{19}\text{F},\alpha\gamma)^{16}\text{O}$  reaction in these targets (in both normal and inverse kinematics). Preliminary results showed unexpectedly large electron-screening values, pointing to a dependence of the electron screening potential on the position of the target nuclei in the metallic lattice.

We have extended our engagement on systems for the detection of ionizing photons and particles at extremely high count rates, both in relation to the construction of the international research facility FAIR in Darmstadt, Germany, as well as in collaboration with domestic and foreign industrial partners, specifically in fields of medical physics and nuclear security. We have started a collaborative characterization of a new type of neutron-detection

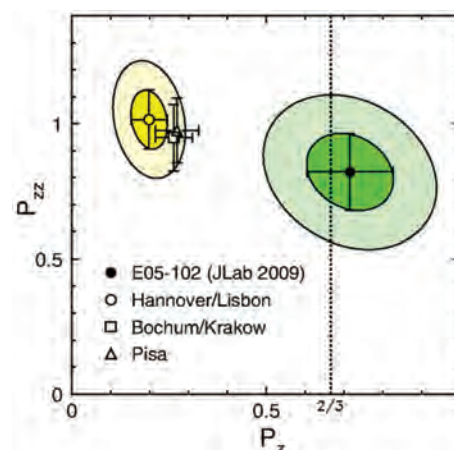


Figure 1: Effective vector and tensor deuteron polarizations (spin orientations)  $P_z$  and  $P_{zz}$  in  $^3\text{He}$  extracted from the data and theoretical predictions at  $p_m \rightarrow 0$  in the approximation of  $e-d$  elastic scattering [with  $1\sigma$  and  $2\sigma$  covariance ellipses on the experiment (green) and the numerically most reliable theory interpolation (H-L, yellow)]. If the spin part of the  $^3\text{He}$  wave function were given simply by a Clebsch-Gordan combination of the proton and deuteron parts, one would expect  $P_z=2/3$  and  $P_{zz}=0$ . From Mihovilović et al., Phys. Rev. Lett. 113 (2014) 232505.

**We published the first paper reporting on our studies of proton and deuteron knock-out from  $^3\text{He}$  (Mihovilović et al., Phys. Rev. Lett. 2014), as well as a paper in Nature on studies of the parity violation in deep inelastic electron-quark scattering (Wang et al., Nature 2014).**



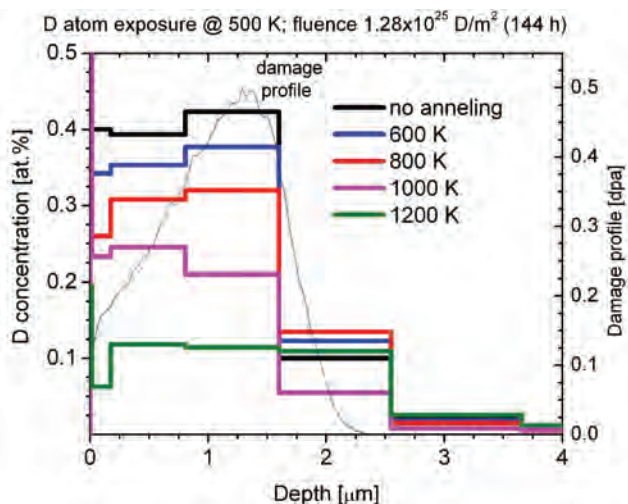


Figure 2: Deuterium concentration depth profiles in structurally damaged tungsten obtained after exposure to atomic deuterium for different annealing temperatures. For higher annealing temperatures the concentration of retained deuterium in the entire damaged layer homogeneously decreased. The defects (dislocations, vacancies) are annealed and recombined at higher temperatures, resulting in a density reduction of the strong binding sites for deuterium (Markelj et al., unpublished).

**In a tough competition, we obtained new beamtime at the free-electron laser FERMI scheduled in 2015, based on a successful earlier beam campaign at FERMI (Žitnik et al., Phys. Rev. Lett. 2014).**

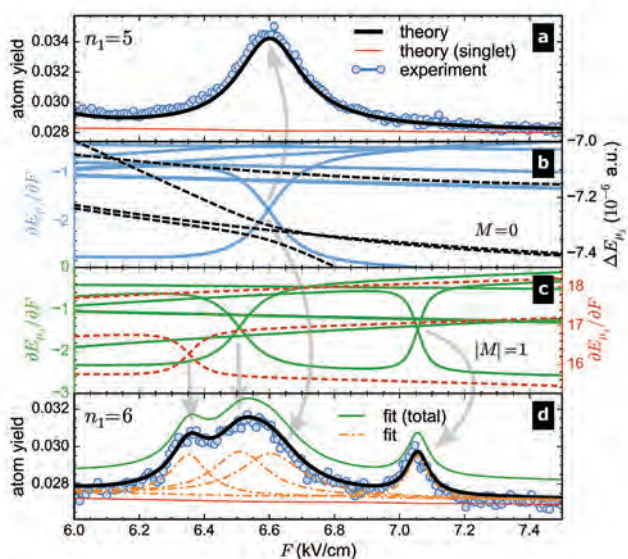


Figure 3: Dependence of the metastable He atoms on the electric field strength at photonic excitation of the group of the atomic states  $1sn11$  (Mihelič et al., PRA 89, 063422, 2014).

material with the US govt. research facility Y12 of Oak Ridge. In February 2014 we closed a deal for the first-ever sale of commercial IP rights on a patent (Vencelj et al, P-201300428) by the JSI. On other research subjects, we have filed for two more patents, one at the London IP Office and the other one in Ljubljana.

The Laboratory for Radioactivity Measurements was conducting the environmental radioactivity monitoring of a living environment in Slovenia, regular Krško Nuclear Power Plant (KNPP) off-site environmental radioactivity monitoring, independent verification of the regular environmental radioactivity monitoring around KNPP, central radioactive waste repository radiological monitoring, monitoring of the radioactivity in drinking water, intercomparisons, proficiency tests, material characterizations, calibrations of the radiation gauges and TLD measurements of the personal and environmental doses.

In the Laboratory for Liquid Scintillation Spectrometry, the frame of accreditation in accordance to SIST EN ISO/IEC 17025 was enlarged in 2014. A new accredited method is the gross alpha/beta determination in different types of waters, recommended as a screening test for water supplies in European Directive 20013 / 51 / EURATOM. A long-term cooperation with Scottish enterprise IARMA was established in the field of the preparation and characterization of reference materials and intercomparison samples. Several samples of water and fuels were analysed for national monitoring programs and other costumers from Slovenia and abroad. Tritium and C-14 are the most commonly determined radionuclides.

In 2014 we continued intensified cooperation with the Metrology Institute of the Republic of Slovenia (MIRS). As the designated institute and as the holder of the national standard in the field of ionizing radiation in Slovenia, we continued the activities on projects from EU funding EMRP research programme: “Metrology of ionising radiation in metallurgical industry” (MetroMetal) and “Metrology for Radioactive Waste Management” (MetroRWM), “Metrology for processing materials with high natural radioactivity (MetroNORM)”. In 2014 we started to work within a new EMRP project “Metrology for radiological early warning networks in Europe” (ENV57 MetroERM). The main deliverable of the group will be the design and construction of a high volume flow-rate air-pump with an embedded spectrometric system for the identification of the radionuclides in the case of an incidental release.

The radiological mobile unit performed its regular preparedness service, as well as in-field preparedness trainings around the Nuclear Power Plant Krško and a demonstration exercise in collaboration with the Administration of the Republic of Slovenia for Civil Protection and Disaster Relief. Part of the personnel took part at RANET exercise in Fukushima, Japan, in November 2014.

At the beginning of 2014, the atomic physics group collaborated with colleagues from Oulu University, Finland, for experiments held at beamline I411 of MaxLab2 facility in Lund, Sweden, where they studied the decay of chloromethanes under the excitation with synchrotron light close to the ionization threshold of the Cl  $L_{23}$  shell (200–210 eV). They measured the yield of Auger electrons L-VV in coincidence with ionic fragments during the variation of the impact photon energy (PEPICO). The spectra were sorted after the type of the final ionic fragment, a type of the experiment not reported so far. The results demonstrated the strong influence of the photon energy

on the final fragment distribution, i.e., the ion  $HCl^+$  is formed exclusively during the decay of the so-called LUMO resonance  $\sigma^*$ , and only in the case of the  $CH_3Cl$  molecule.

The atomic physics group published two papers dealing with the decay of CHC molecules after the formation of the vacancy in the K shell of a chlorine atom, studied with Resonant Inelastic X-Ray Scattering (RIXS). In the first paper we show that in the initial phase of dissociation the bond between the Cl atom and its adjoint atom (C,

H, Cl) is stretched (Bohinc et al., Jour. Chem. Phys., 2014). In the second paper, the iso- $C_2H_2Cl_2$  is studied with the RIXS Cl K-L method (Kawerk et al., Jour. Chem. Phys., 2014). In collaboration with a group from Stanford University, high-resolution measurements of the spectral maps were executed by RIXS at the SSRL synchrotron for the energies of double excitations  $1s4p$  and  $1s3d$  in Kr. With the analysis of the hard X-ray spectra we isolated the signals of two-electron excitations up to their energy threshold and compared the results with an earlier arbitrary separation based on the photoabsorption signal (Kavčič et al., Phys. Rev. A, 2014). The last results of the research group at the field of high-energy resolution X-ray spectroscopy are reported in a review article (Žitnik et al., Jour. Phys.: Conf. Ser. 2014).

In the field of high-energy-resolution proton-induced x-ray spectroscopy (HR-PIXE) we have performed in 2014 at the Microanalytical center systematic measurements of  $K\alpha$  and  $K\beta$  characteristic x-ray emission spectra from the representative set of phosphorus-, sulphur-, and chlorine-containing compound targets. Due to very high experimental resolution on the level of natural K level broadening of the studied elements the measured spectra exhibit pronounced chemical bonding effects and yield an opportunity to study the local chemical environment. In combination with advanced quantum chemistry computational methods based on the density functional theory these measurements set the ground base for the quantitative bulk analysis of electronic structure of low Z materials by using x-ray emission spectroscopy. In collaboration with the group from the University of Guelph, Ontario, Canada, led by Prof. Campbell, we have performed high-resolution PIXE measurements of Si and  $SiO_2$  targets induced by 3–5 MeV He ions. The measurements will make it possible to study KL double ionization and chemical bonding effects on the K shell fluorescence yields in Si oxides, which limits the accuracy of silicate rocks PIXE analysis. Besides HR-PIXE measurements, in 2014 we have also performed characterization measurements of the polycapillary x-ray collimating optics at the IfG institute in Berlin. This polycapillary X-ray optics will be used in the design of the new x-ray emission spectrometer that will combine the collimating X-ray optics and Bragg diffraction on a flat crystal. The use of X-ray optics will drastically enhance the X-ray collection efficiency, while the energy resolution defined by the small divergence of the X-rays exiting the polycapillary semi lens will reach 10–20 eV, which will significantly improve the sensitivity and lower the detection limits of the micro PIXE analysis.

In 2014, we started joint experimental work with the Laboratory for Quantum Optics at the University in Nova Gorica. We used the laser VUV light emitted by a neon gas target excited by a strong laser at a wavelength of 800 nm. We figured out that the energy of 39. harmonics HHG approaches double excited state  $He\ 2^+ \ ^1P_0$  at 60.15 eV and that the available photon flux allows for the execution of a two-colour experiment. This resonance would serve us as a starting point, from which we will be able to excite the He atoms in other resonant states with an additional pulse of laser infrared light.

At the Soleil synchrotron we executed experiments, at which we measured spectra of transitions, where double inner shell vacancy is filled with a pair of electrons, and the third electron is ejected as an Auger electron. It turned out that such a transition of the three electrons involved is significantly imprinted in the spectra in spite of the dominant cascade decay of the double-vacancy state, where two consecutive Auger electrons are ejected. In the autumn of 2014 we participated at the magnetic bottle experiments at the synchrotron Soleil, beamline Sextant in collaboration with University Paris 6. A high detection efficiency of the magnetic bottle was used in attempts of the detection of the process, where a single photon absorption in the shell L of Ar results in the creation of three vacancies.

At the end of 2014 we performed two experiments on the Gasphase beamline at the Elettra synchrotron facility. The first was dedicated to VUV spectrometry in the direction of the incoming photon beam and to the measurements of the density of the gas that is released during short opening of the Even-Lavie valve into the vacuum chamber. Both experiments were dedicated to the preparation for the experiment "Amplified VUV emission from Doubly Excited Helium Atoms" approved in 2014 at free-electron

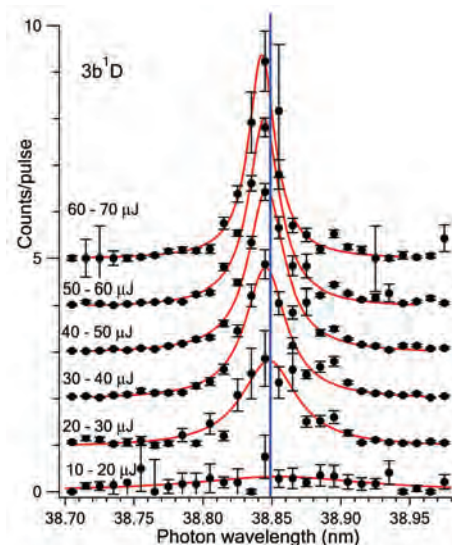


Figure 4: Dependence of spectral line shape of even resonance  $1De$  in He on the energy of impact laser pulse at the photon excitation in the energy range 32.95 - 33.20 eV at free-electron laser FERMI (Žitnik et al., PRL 113 (2014) 193201).

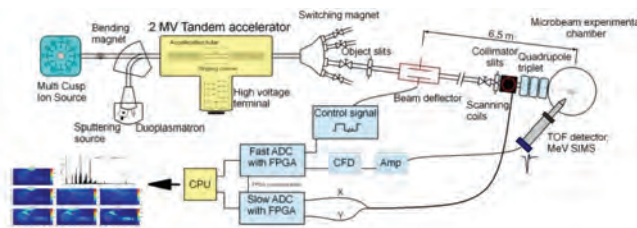


Figure 5: Schematic view of the MeV SIMS system at the ion accelerator of the Jožef Stefan Institute (Jeromel et al., unpublished).

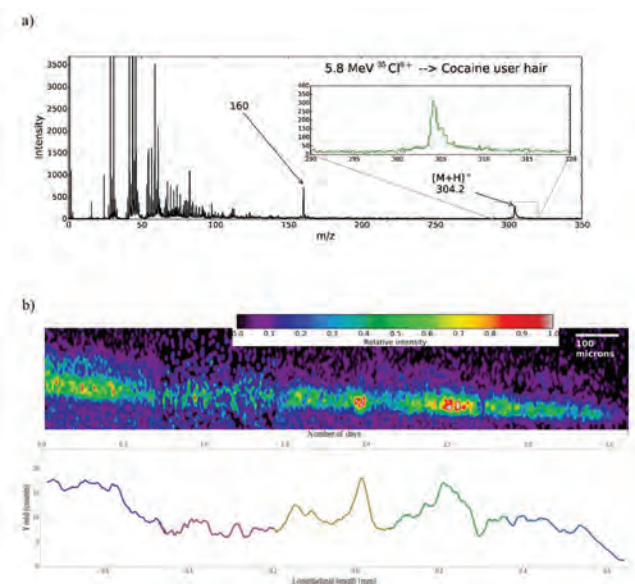


Figure 6: (a) MeV SIMS spectra measured at the hair sample of cocaine user. A 5.8-MeV  $^{35}Cl_6^+$  beam was used as excitation source. (b) Map and extracted longitudinal profile of the yield in the cocaine peak at an  $m/z$  of 304 u along 1.4 mm of the hair, corresponding to approx. 3.5 days of hair growth (Jeromel et al., unpublished).



**In 2014, we demonstrated that the tritium retained in the divertor area of ITER, consisting of structurally damaged tungsten due to neutron damage, could be cleaned by exposure to atomic hydrogen beams via an isotope-exchange process. By in-situ Nuclear Reaction Analysis (NRA), we predicted the temperature threshold for the successful cleaning, as well as the quantitative rates of tritium removal.**

laser Fermi in tough international competition. We published a paper on the experiment at Fermi dedicated to the first two-photon high-resolution spectroscopy in the VUV energy region on a free-electron laser. Through the detection of metastable atoms, we were able to detect energy shifts of spectral lines of few meV (Žitnik et al., Phys. Rev. Lett. 2014). In December 2014 we performed a “Stark” experiment at Elettra with new compact high-resolution spectrometer for VUV light and measured the fluorescence of doubly-excited states in He in an electric field with a strength of up to 20 KV/cm. With this experiment we continued the research on the behaviour of He in strong electric and magnetic fields. In 2014 we also published two articles on this topic (Mihelič et al., Phys. Rev. A, 2014 and Bučar et al., Phys. Rev. A, 2014).

The material properties were studied with measurements of magnetic and electric hyperfine fields using Mössbauer spectroscopy. The research was focused on cathode materials for lithium batteries, which were studied at the synchrotron facilities Petra in Hamburg and APS in Chicago. The sample structure was revealed by X-ray diffraction techniques, neutron diffraction, Mössbauer spectroscopy using  $^{57}\text{Fe}$  isotope and NMR spectroscopy on  $^6\text{Li}$ . Based on these results we presented a model “1Fe 2Li” on the cation distribution in  $\text{LiFeBO}_3$ . We have investigated the properties of superparamagnetic maghemite nanoparticle clusters using X-ray diffraction, TEM, Mössbauer spectroscopy in external magnetic field and magnetic measurements.

The group for x-ray absorption spectroscopy gained collaboration beamtimes at two synchrotron facilities ESRF (Grenoble) and Elettra (Trieste), and performed five experiments of one week each. In collaboration with the Institute for Chemistry, Ljubljana a series of *in-operando* XANES and EXAFS experiments on high-energy-density Li-sulphur batteries with modified cathode materials and electrolyte without sulphur were performed. The XAS spectra were recorded during charging and discharging of the battery. In this way we were able to monitor with high precision the change of the valence of sulphur, and the formation of Li-polysulphides ( $\text{Li}_2\text{S}_x$ ) compounds and finally crystalline  $\text{Li}_2\text{S}$  during discharge, and reversibility of the process during charging, i.e., the key information on the battery dynamics which opened the way to optimization of the synthesis of the material with maximum capacity (Urbani et al, Chem. Phys. Chem. 2014).

In collaboration with Biotechnical Faculty of University of Ljubljana, Université catholique de Louvain (Belgium), Universitaet Bayreuth (Germany), ESRF Grenoble (France), National Agri-Food Biotechnology Institute (Mohali, India), we performed XAS experiments to determine the distribution of pollutant elements (Se, Hg, Cd, Pb) and essential elements (Zn, Cu, Ni, Mn, Fe) at the cellular level. We published the analysis of Cd and Zn binding at the cellular and tissue level (Lefevre et al, Plant, cell, environ., 2014). The distribution of sulphur, chlorine and zinc was scanned simultaneously to reveal correlations between the elements and micro-XANES to elucidate chemical bonding of the elements in different parts of the cells.

In collaboration with the Laboratory for Material Research of the University in Nova Gorica we published two papers about the cation order-disorder transition in Fe-doped  $6\text{H-BaTiO}_3$  for dilute room-temperature ferromagnetism (Mikulska et al, Jour. Amer. Cer. Soc., 2014). The Fe EXAFS and XANES revealed the source of ferromagnetism in the crystal structure of the  $\text{Fe}_3^+$ -doped material. We continued a long-term project in collaboration with the Institute of Chemistry, which involves XAS measurements on the catalytic mesoporous molecular sieves doped with Ca, Ti Cr, Mn, Fe, Ni and Cu, also containing organic building units and on CuPd catalysts. The valence of

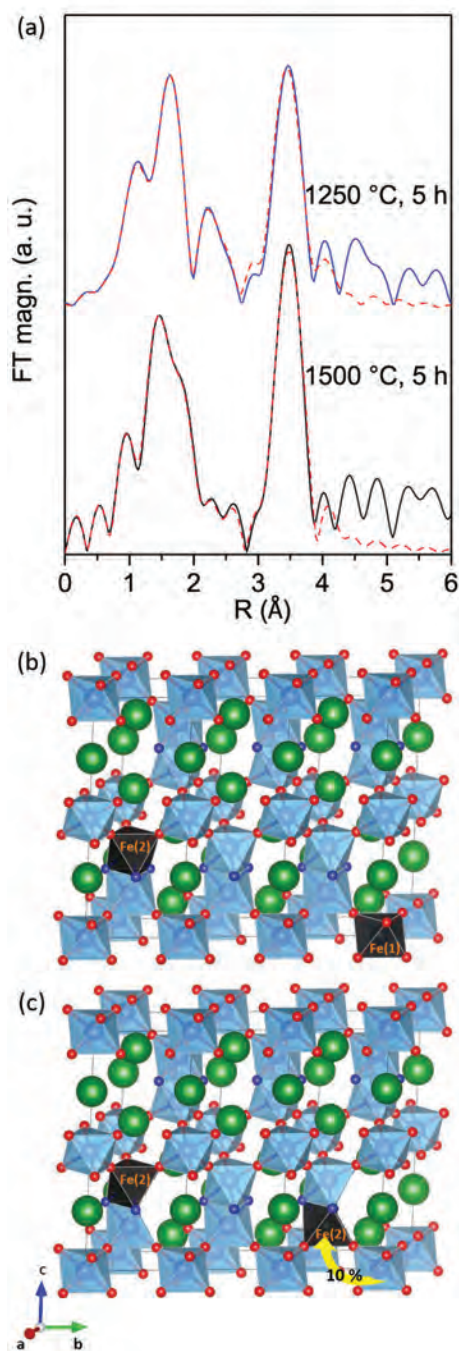


Figure 7: (a) The Fourier-transform magnitudes of 10% Fe-doped  $\text{BaTiO}_3$  annealed at different temperatures (dashed line - best fit EXAFS model). (b) and (c) Schematic view of the Fe-distribution within three unit cells of the Fe-doped  $6\text{H-BaTiO}_3$  crystal structure (space group  $P63/mmc$ ): (b) after treatment at  $1250^\circ\text{C}$  for 5 h, (c) additionally annealed at  $1500^\circ\text{C}$  for 10 h. The polyhedra represent octahedrally coordinated Ti atoms. The Fe atoms incorporated onto  $\text{Ti}(1)$  and  $\text{Ti}(2)$  sites and their coordination octahedra are marked black. The octahedra with missing faces illustrate the oxygen vacancy in the corresponding face-sharing plane. The large spheres are Ba atoms. The dark and light smaller spheres are oxygen atoms on the  $\text{O}(2)$  and  $\text{O}(1)$  crystallographic sites, respectively. The arrow marks the movements of  $\text{Fe}^{3+}$  from  $\text{Ti}(1)$  sites to  $\text{Ti}(2)$  sites after additional annealing at  $1500^\circ\text{C}$  for 10 h. (Mikulska et al., Jour. Amer. Ceramic Soc. 2014,1)

dopants and their atomic neighbourhood is determined to elucidate their catalytic properties (Jevtić et al, *Microp. mesopor. mat.*, 2014).

At the ion accelerator we intensively used the micro-PIXE method for selected biology research problems in collaboration with Biotechnical Faculty, University of Ljubljana (BF UL). The efforts invested in the last years to optimize the proton beam quality from the multicusp ion source came into the frontline, as the ion source provides the H beam with the highest ever reported proton beam brightness at the tandem accelerators worldwide (Pelicon et al, *Nucl. Instr. Meth. B*, 2014). For the micro-PIXE measurements we managed to form a 3-MeV proton beam with a diameter of 700 nm, which allows excellent elemental mapping in biological materials. We established a methodology for the quantification of elemental mass inventories in single-cell biological systems with a precision of 1 pg ( $10^{-12}$  g). With this method, we investigated the uptake of gold nanoparticles in human dendritic cells in collaboration with Military Academy Hospital in Belgrade (Tomić et al, *Plos One*, 2014). In collaboration with BF UL and National Agri-Food Biotechnology Institute, Mohali, India, we published the results on the iron in wheat grains (Singh et al, *Planta* 2014). Further steps toward routine use were made with frozen hydrated tissue processing for micro-PIXE.

Important advances were seen for the development of the MeV SIMS method, where we completed the acquisition system of desorbed molecules in the imaging mode. We applied a  $^{35}\text{Cl}^{6+}$  ion beam with an energy of 5.8 MeV. We measured molecular maps of the desorbed molecular ions in tea-leaf cross-sections, as well as over the cross-section of the wheat grains. In collaboration with the institute Amolf, Amsterdam, we measured the distribution of cocaine along the hair of the drug user, which reflects the changes of the physiological concentrations in the blood of the user on a scale of 1 hour.

Fusion research at the ion accelerator was coordinated within the Work Package on "Preparation of efficient Plasma-Facing Component (PFC) operation for ITER and DEMO" (WP PFC). Our main focus was to study: i) the role of neutron damage on the fuel retention mechanism in tungsten and ii) isotope exchange capabilities of ITER and DEMO materials. Work was performed in collaboration with IPP, Garching, Germany, who prepared W samples and produced neutron-like damaged tungsten by bombardment with high-energy 20-MeV W ions. In the first task we have studied the temperature dependence of trap formation in self-damaged W, where samples after damaging at room temperature were annealed at temperatures from 300 to 1200 K and then loaded with atom beam for 144 h (D fluence  $1.3 \times 10^{25}$  D/m<sup>2</sup>) at 500 K. The atoms decorate the defects, which are acting as additional strong binding sites for deuterium atoms in the bulk, without producing any additional damage. By analysing the deuterium depth profile by Nuclear Reaction Analysis (NRA) (employing the  $\text{D}(^3\text{He},\text{p})\alpha$  nuclear reaction) in such treated samples, we have studied the effect of sample heating on the damage annealing. The annealing temperature was found to have a strong influence on the maximum concentration of deuterium in the damaged layer of the material. For the second task we studied hydrogen isotope exchange in self-ion damaged tungsten. Fuel retention and its removal by isotope exchange was studied by in-situ NRA (Markelj et al., *Phys. Scr.* 2014). During the exposure of the sample to the atomic deuterium beam, the deuterium concentration depth profiles were measured, obtaining the deuterium migration dynamics into the material and removal dynamics during the isotope exchange at 600 K. The isotope exchange was efficient in both cases, with the conclusion that isotope exchange in self-damaged W is efficient by neutral hydrogen atoms at 600 K and therefore being a possible tritium-removal method.

In the field of archaeometry with Ion Beam Analysis we investigated semiprecious stones, glass and metals. We completed our research of garnets from the sites of the Migration period. According to their composition measured by the PIXE-PIGE method, the garnets originate from the sites of South India and Sri Lanka. Among the investigation of glass, we completed a study of glass beads from the Greek city of Apollonia Pontica in present Bulgaria. It was shown that the beads dated between 5<sup>th</sup> and 3<sup>rd</sup> century BC were made of glass made of Egyptian natron, and were very likely produced in one of the major Greek glassworks, possibly on the island of Rhodes. The studies of metals involve consideration of brass-made scabbards in Late Iron Age style. It was argued that the artefacts were produced in Roman workshops in a manner that pleased Roman barbaric allies who received them as diplomatic gifts. On the Iron Age ceramics we identified the white pigments as tin oxide. In the field of inner-shell ionization we warned about correct calculation of ECPSR cross-sections that form a basis for the concentration-evaluation

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**We completed the in-house development of the MeV SIMS method at the JSI tandem accelerator. During the first analytical trials, we managed to map the presence of cocaine in the hair of a cocaine user with a lateral resolution corresponding to a hair growth period of 1 hour.**

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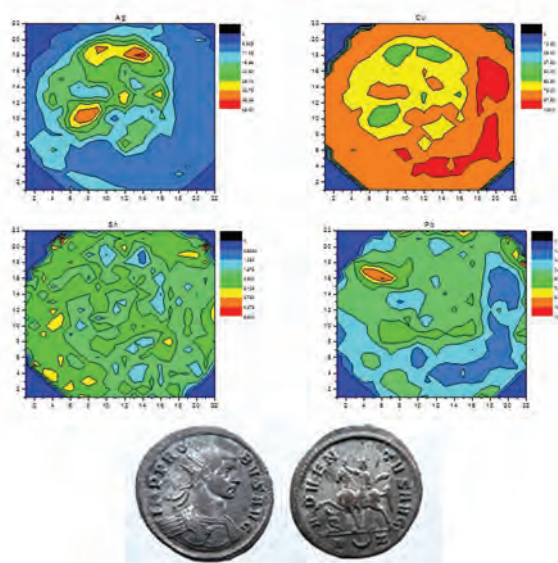


Figure 8: Elemental mapping of the Roman silver coin Probus by in-air PIXE (Fajfar et al., unpublished).



algorithms in PIXE. As a new development of the in-air beamline at the Tandemtron accelerator we developed a system for the scanning mode of measurement and generation of concentration maps. Our first measurements involve studies of plated materials, mainly plated and surface-enriched silver coins and gilded bronzes.

## Some outstanding publications in the past year

1. Wang et al., *Nature* 506 (2014) 67
2. Mihovilovič et al., *Phys. Rev. Lett.* 113 (2014) 232505.
3. Lefevre et al, Plant, *Cell & Env.* 37 (2014), 1299–1320
4. Žitnik, M., Mihelič, A., Bučar, K., Kavčič, M., et al., *Phys. Rev. Lett.* 113 (2014), 193201
5. Bohinc, R., Žitnik, M., Bučar, K., Kavčič, M., *The Journal of chemical physics* 140 (2014), 164304
6. Tao, L., Roussel, G., Chotard, J. N., Dupont, L., Bruyère, S., Hanžel, D., Mali, G., Dominko, R., Levasseur, S., Masquelier, C., *Journal of materials chemistry: A, Materials for energy and sustainability* 2 (2014), 2060
7. Batra, A., Kladnik, G., Gorjizadeh, N., Meisner, J. S., Steigerwald, M., Nuckolls, C., Quek, S. Y., Cvetko, Dean, Morgante, A., Venkataraman, L., *Journal of the American Chemical Society* 136 (2014), 12556
8. Kokalj, T., Park, Y. G., Vencelj, M., Jenko, M., Lee, L. P., *Lab on a chip* 14 (2014), 4329

## Organization of conferences, congresses and meetings

1. BioPIXE8, Bled, Slovenia, 14–19 September 2014

## INTERNATIONAL PROJECTS

1. TLD Dosimetry  
Boštjan Črnič  
Foreign buyers
2. Calibrations  
Matjaž Mihelič, M. Sc.  
Foreign buyers
3. Provision of Testing Services for Filter Media used in IMS Radionuclide Stations  
Dr. Benjamin Zorko  
The Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization
4. Small Services  
Dr. Marijan Nečemer  
Foreign buyers
5. Micro-PIXE: Plant Sample Analysis  
Prof. Primož Pelicon  
Foreign buyers
6. 7FP - SPRITE; Supporting Postgraduate Research with Internships in Industry and Training Excellence  
Asst. Prof. Matjaž Kavčič  
European Commission
7. 7FP - PREPARE; Innovative Integrative Tools and Platforms to be Prepared for Radiological Emergencies and Post-accident Response in Europe  
Dr. Benjamin Zorko  
European Commission
8. 7FP - EURATOM-MHEST, WP13-IPH-A03-P1-01/MESCS/PS, Atomic and Low-Energy Hydrogenic Plasma Interaction with Damaged Tungsten  
Dr. Sabina Markelj  
Ministry of Education, Science and Sport
9. 7FP - EURATOM-MHEST, WP13-IPH-A03-P2-01/MESCS/PS, D Re-Adsorption/Re-Saturation of W Surfaces Subject to Helium RF - Discharge as a Fuel Removal Technique  
Dr. Sabina Markelj  
Ministry of Education, Science and Sport
10. MetroRWM; Metrology for Radioactive Waste Management  
Branko Vodenik, M. Sc.  
Euramet e.V.
11. MetroMetal - Ionising Radiation Metrology for the Metallurgical Industry  
Branko Vodenik, M. Sc.  
Euramet e.V.
12. COST CM1204: XUV/X-ray Light and Fast Ions for Ultrafast Chemistry (XLIC)  
Prof. Matjaž Žitnik  
COST Office
13. Hydrogen Retention in Self-damaged and He Irradiated Tungsten Alloys in Fusion Devices; Plasma-Wall Interaction for Irradiated Tungsten and Tungsten Alloys in Fusion Devices  
Dr. Sabina Markelj  
IAEA - International Atomic Energy Agency
14. RC 18186/R0; Application of Synchrotron Radiation in Studies of Environmental Impact on Biological Organisms; Experiments with Synchrotron Radiation for Modern Environmental and Industrial Applications

- Dr. Peter Kump  
IAEA - International Atomic Energy Agency
15. MetroNORM; Metrology for Processing Materials with High Natural Radioactivity  
Branko Vodenik, M. Sc.  
Euramet e.V.
16. RC 18353/R0; Dual Imaging of Biological Samples with MeV SIMS and PIXE Analysis; Development of Molecular Concentration Mapping Techniques using MeV Focussed Ion Beams  
Prof. Primož Pelicon  
IAEA - International Atomic Energy Agency
17. MetroERM; Metrology for Radiological early warning networks in Europe  
Denis Glavič Cindro, M. Sc.  
Euramet e.V.
18. IAEA Fellowships for Mr. Javier Flores Maldonado, (MEX 14008V), Ms. Francisca Aldape de Flores (MEX 14009V) and Ms. Elizabeth Vega-Rangel (MEX 14010V), 14-19 September 2014  
Prof. Primož Pelicon  
IAEA - International Atomic Energy Agency
19. Virtual Compton Scattering on the Nucleon  
Prof. Simon Širca  
Slovenian Research Agency
20. Study of Deeply Virtual Compton Scattering  
Prof. Simon Širca  
Slovenian Research Agency
21. Double Core Hole Formation by Photon and Proton Impact  
Prof. Matjaž Žitnik  
Slovenian Research Agency
22. Molecular Imaging of Biological Samples Using MeV Ions and keV Clusters for TOF-SIMS Spectrometry  
Prof. Primož Pelicon  
Slovenian Research Agency
23. Plasma Facing Components-1-IPH-FU, EUROFUSION  
Dr. Sabina Markelj  
European Commission
24. Education-ED-FU, EUROFUSION  
Prof. Primož Pelicon  
European Commission

## RESEARCH PROGRAMS

1. Structure of Hadronic Systems  
Prof. Simon Širca
2. Studies of Atoms, Molecules and Structures by Photons and Particles  
Prof. Matjaž Žitnik
3. Object and Prestige; Taste, Status, Power (Researches of the Material Culture in Slovenia)  
Dr. Marijan Nečemer
4. Archaeological and Archaeometric Research of Portable Archaeological Heritage  
Prof. Žiga Šmit

## R & D GRANTS AND CONTRACTS

- Investigation of Plant Ion Homeostasis using Elemental Imaging by Laser Ablation - Inductively Coupled Plasma Mass Spectrometry (Basic Research Project)  
Prof. Primož Pelicon
- Research of the Ionome of Selected Mycorrhizal Plants  
Prof. Primož Pelicon
- Nanostructured Cathodes for Lithium Sulphur Batteries  
Dr. Darko Hanžel
- Sustainable Land Use in Relation to Soil and Crop Quality  
Prof. Primož Pelicon
- Archaeologies of Hunter-gatherers, Farmers and Metallurgists: Cultures, Populations, Palaeoeconomies and Climate  
Dr. Marijan Nečemer
- Vegetation and Hydrology of Ljubljansko barje in the Past, Present and Future - a Consequence of Succession, Human Impact or Climatic Fluctuations?  
Dr. Marijan Nečemer
- 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
- Evaluation of Quality and Safety Parameters of Vegetables Produced on Different Systems in Slovenia and Abroad with Aim to Establish National Quality Scheme for Vegetables  
Dr. Marijan Nečemer
- Center of Competence BioMedical Engineering: CC BME  
Dr. Matjaž Vencelj
- Electron Screening in Metals  
Dr. Jelena Vesic
- 8th International Symposium on Bio-PIXE (Bio-PIXE 8), Bled, Slovenia, 14-19 September 2014  
Prof. Primož Pelicon

## NEW CONTRACTS

- Annex No. 9 to the Contract on Performing Activities and Fulfillment of Obligations of Holder of National Standard in the Field of Ionising Radiation  
Matjaž Mihelič, M. Sc.  
Ministry of Higher Education, Science and Technology
- Radiological Analysis of Groundwater, Soil and Rocks in the Main Researches of the Geosphere and Hydrosphere in Light of Construction of the LILW Repository  
Dr. Benjamin Zorko  
National Laboratory of Health, Environment and Food
- Maintenance of Radiological Emergency Preparedness for a Period of 5 Years (2012-2017)  
Asst. Prof. Matej Lipoglavšek  
Krško Nuclear Power Plant
- Extension of MPPC Performance into the Saturation Regime  
Dr. Matjaž Vencelj  
Beyond Devices, d. o. o.
- Environmental Radioactivity Monitoring of Living Environment in Republic of Slovenia for 2013 and 2014  
Dr. Benjamin Zorko  
Ministry of Agriculture, Forestry and Food
- Regular Krško Nuclear Power Plant Off-site Environmental Radioactivity Monitoring for 2014 and 2015  
Dr. Benjamin Zorko  
Krško Nuclear Power Plant
- Monitoring of the Radioactivity in Drinking Water in Republic of Slovenia in 2014  
Dr. Benjamin Zorko  
Ministry of Health
- Monitoring of Central LILW Storage Facility at Brinje 2014  
Dr. Marijan Nečemer  
ARAO
- Sale and Transfer of Intellectual Property Rights Share over a Joint Invention  
Dr. Matjaž Vencelj  
Instrumentation Technologies, d. d.

## VISITORS FROM ABROAD

- Prof. Ron M. A. Heeren, AMOLF, Amsterdam, Netherlands, 22-25 January 2014
- Dr. Antti Hakkola, VTT Technical research Centre, Espoo, Finland, 1-2 April 2014
- Dr. Thomas Schwartz-Selinger, IPP, Garching, Germany, 1-2 April 2014
- Michele Di Fraia, B. Sc., Elettra, Trieste, Italy, 20 February-20 July 2014
- Abdulghani Shakhshiro, IARMA, Vienna, Austria, 28-31 March 2014
- Dr. Klaus Gross, GSI, Darmstadt, Germany, 30 March-1 April 2014
- Dr. Karlheinz Langanke, GSI, Darmstadt, Germany, 30 March-1 April 2014
- Dr. Régis Bisson, Aix Marseille Université, Marseille, France, 5-7 May 2014
- Othmen Saidi, Aix Marseille Université, Marseille, France, 5-9 May 2014
- Dr. Yves Ferro, Aix Marseille Université, Marseille, France, 6-8 May 2014
- Dr. Helene Fonville, CNRS, LPC Clermont-Ferrand, Clermont-Ferrand, France, 20-25 July 2014
- Loup Correa, CNRS, LPC Clermont-Ferrand, Clermont-Ferrand, France, 20-25 July 2014
- Josef Buchriegler, HZDR, Dresden, Germany, 11 September-13 October 2014
- Dr. Chris Heirwegh, University of Guelph, Guelph, Canada, 29 September-3 October 2014
- Dr. Irina Pradler, University of Guelph, Guelph, Canada, 29 September-3 October 2014
- Dr. Jolanta Mesjasz Przybylowicz, NRF, iThemba LABS, Somerset West, South African Republic, 2-7 October 2014
- Dr. Wojciech Przybylowicz, NRF, iThemba LABS, Somerset West, South African Republic, 2-7 October 2014
- Dr. Francis Penet, LCPMR, Paris, France, 13-21 November 2014
- Amelie Betzlbacher, University of Bayreuth, Bayreuth, Germany, 23-27 November 2014
- Stephan Höreth, University of Bayreuth, Bayreuth, Germany, 23-27 November 2014
- Dr. Paula Pongrac, University of Bayreuth, Bayreuth, Germany, 23-27 November 2014
- Dr. Isabelle Lefevre, Biology centre ASCR, České Budějovice, Czech Republic, 26 November-17 December 2014
- Dr. Pascal Lablanquie, LCPMR, Paris, France, 8-14 December 2014
- Dr. Lidija Andrić, Université Pierre et Marie Curie, Paris, France, 10-14 December 2014

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- Dr. Klemen Bučar
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- Denis Glavič Cindro, M. Sc.
- Dr. Darko Hanžel
- Asst. Prof. Matjaž Kavčič
- Dr. Jasmina Kožar Logar
- Dr. Peter Kump
- Asst. Prof. Matej Lipoglavšek
- Dr. Sabina Markelj
- Dr. Andrej Mihelič
- Dr. Marijan Nečemer
- Prof. Primož Pelicon, Head**
- Zdravko Rupnik, M. Sc.
- Prof. Simon Širca\*
- Prof. Žiga Smit\*
- Dr. Matjaž Vencelj
- Branko Vodenik, M. Sc.
- Dr. Benjamin Zorko
- Prof. Matjaž Žitnik

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- Dr. Toni Petrovič
- Dr. Jelena Vesic

### Postgraduates

- Jure Beričič, B. Sc.
- Rok Bohinc, B. Sc., left 01. 05. 14*
- Tilen Brecelj, B. Sc.
- Boštjan Jencič, B. Sc.
- Luka Jeromel, B. Sc.
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- Nina Ogrinc Potočnik, B. Sc., on leave 01. 06. 14*
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- Technical and administrative staff**
- Drago Brodnik
- Mojca Gantar
- Sandi Gobec
- Zvonimir Grabnar, retired 01. 12. 14*
- Mirko Ribič, B. Sc.

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

1. A1 Collaboration, J. C. Bernauer *et al.* (25 authors), "Electric and magnetic form factors of the proton", *Phys. rev. C. Nucl. phys.*, vol. 90, iss. 1, pp. 015206-1-015206-34, 2014.
2. A1 Collaboration, Harald Merkel *et al.* (36 authors), "Search at the Mainz microtron for light massive gauge bosons relevant for the muon g - 2 anomaly", *Phys. rev. lett.*, vol. 112, iss. 22, pp. 221802-1-221802-5, 2014.
3. S. Abrahamyan *et al.*, "New measurements of the transverse beam asymmetry for elastic electron scattering from selected nuclei", *Phys. rev. lett.*, vol. 109, no. 19, pp. 192501-1-192501-6, 2014.
4. Arunabh Batra, Dean Cvetko, Gregor Kladnik, Olgun Adak, Claudia Cardoso, Andrea Ferretti, Deborah Prezzi, Elisa Molinari, Alberto Morgante, Latha Venkataraman, "Probing the mechanism for graphene nanoribbon formation on gold surfaces through X-ray spectroscopy", *Chem. sci.*, vol. 5, iss. 11, pp. 4419-4423, 2014.
5. Arunabh Batra, Gregor Kladnik, Narjes Gorjizadeh, Jeffrey S. Meisner, Michael Steigerwald, Colin Nuckolls, S. Y. Quek, Dean Cvetko, Alberto Morgante, Latha Venkataraman, "Trimethyltin-mediated covalent gold-carbon bond formation", *J. Am. Chem. Soc.*, vol. 136, iss. 36, pp. 12556-12559, 2014.
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7. Ljudmila Benedik, G. Sibbens, Adrian Moens, Roger Eykens, Marijan Nečemer, Srečo D. Škapin, Peter Kump, "Preparation of thick uranium layers on aluminium and stainless steel backings", In: Proceedings of the 19th International Conference on Radionuclide Metrology and its Applications, 17-21 June 2013, Antwerp, *Appl. radiat. isotopes*, vol. 87, pp. 238-241, 2014.
8. Rok Bohinc, Matjaž Žitnik, Klemen Bučar, Matjaž Kavčič, "Dissociation dynamics of simple chlorine containing molecules upon resonant  $ClK - \sigma^*$  excitation", *J. chem. phys.*, vol. 140, no. 16, pp. 164304-1- 164304-7, 2014.
9. Klemen Bučar, Matjaž Žitnik, Andrej Mihelič, F. Penent, P. Lablanquie, J. Palaudoux, L. Andric, M. Braune, R. Püttner, "Quenching of the  $2pnd^1P^o$  doubly excited states of helium by a dc electric field", *Phys. rev. A*, vol. 90, no. 1, pp. 013412-1- 013412-7, 2014.
10. Hamdi El-Jendoubi, Saúl Vázquez, Ángele Calatayud, Primož Vavpetič, Katarina Vogel-Mikuš, Primož Pelicon, Javier Abadía, Anunciación Abadía, Fermín Morales, "The effects of foliar fertilization with iron sulfate in chlorotic leaves are limited to the treated area: a study with peach trees (*Prunus persica* L. Batsch) grown in the field and sugar beet (*Beta vulgaris* L.) grown in hydroponics", *Front. plant sci.*, vol. 5, no. 2, pp. 1-16, 2014.
11. S. Fadida, P. Shekhter, Dean Cvetko, Luca Floreano, Alberto Verdini, L. Nyns, S. Van Elshocht, I. Kymissis, Moshe Eizenberg, "Direct observation of both contact and remote oxygen scavenging of  $GeO_2$  in a metal-oxide-semiconductor stack", *J. appl. phys.*, vol. 116, no. 16, pp. 164101-1-164101-6, 2014.
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13. Robert Hauko, Jana Padežnik Gomilšek, Iztok Arčon, Alojz Kodre, "Absolute determination of the X-ray absorption coefficient of strontium in the K edge region", *Radiat. phys. chem.* (1993), vol. 103, pp. 203-208, Oct. 2014.
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18. Jefferson Lab Hall A Collaboration, Y. Zhang *et al.*, "Measurement of "pretzelosity" asymmetry of charged pion production in semi-inclusive deep inelastic scattering on a polarized  $^3He$  target", *Phys. rev. C. Nucl. phys.*, vol. 90, iss. 5, pp. 055209-1-055209-6, 2014.
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24. Matjaž Kavčič, Matjaž Žitnik, Dimosthenis Sokaras, T. -C. Wng, R. Alonso-Mori, D. Norlund, J.-Cl. Dousse, J. Hozzowska, "High-resolution x-ray-emission study of  $1s4p$  and  $1s3d$  two-electron photoexcitations in Kr", *Phys. rev. A*, vol. 90, no. 2, pp. 022513-1-022513-8, 2014.
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- physiological impact in the leaves of the accumulating *Zygophyllum fabago* L.", *Plant cell environ.*, vol. 37, no. 6, pp. 1299-1320, 2014.
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## REVIEW ARTICLE

1. Matej Lipoglavšek, Simon Širca, "Nuclear Physics at Jožef Stefan Institute", *Nucl. phys. news*, vol. 24, no. 4, pp. 28-31, 2014.

## SHORT ARTICLE

1. Paula Pongrac, Ivan Kreft, Katarina Vogel-Mikuš, Marjana Regvar, Mateja Germ, Primož Vavpetič, Nataša Grlj, Luka Jeromel, Diane Eichert, Bojan Budič, Primož Pelicon, "Relevance for food sciences of quantitative spatially resolved element profile investigations in wheat (*Triticum aestivum*) grain", *Excellent in science ...*, pp. [5], 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. A1 Collaboration, Miha Mihovilovič *et al.*, "Initial state radiation experiment at MAMI", In: *International Symposium Lepton and Hadron Physics at Meson-Factories, Messina, Italy, October 13-15, 2013*, (EPJ Web of conferences, vol. 72, 2014), G. Giardina, ed., Les Ulis, EDP Sciences, 2014, pp. 00017-p.1-00017-p.6.
2. A1 hypernuclear collaboration, Sho Nagao *et al.*, "Hypernuclear decay pion spectroscopy at Mainz Microtron", In: *Proceedings of the 12th Asia Pacific Physics Conference, APPC12, July 14-19, 2013, Makuhari, Japan*, (JPS Conference Proceedings, vol. 1), Mamiko Sasao, ed., [Tokyo], Physical Society of Japan, cop. 2014, pp. 013079-1-013079-5.
3. A1 hypernuclear collaboration, A. Esser *et al.*, "Kaon tagging at 023 scattering angle for high-resolution decay-pion spectroscopy", In: *International Nuclear Physics Conference, INPC 2013, Firenze, Italy, June 2-7, 2013*, (EPJ web of conferences, vol. 66, 2014), S. Lunardi, ed., Les Ulis, EDP Sciences, 2014, pp. 11011-p.1-11011-p.5.
4. A1 hypernuclear collaboration, K. Tsukada *et al.*, "Recent studies of the strangeness physics at MAMI-C", In: *Proceedings of the 12th Asia Pacific Physics Conference, APPC12, July 14-19, 2013, Makuhari, Japan*, (JPS Conference Proceedings, vol. 1), Mamiko Sasao, ed., [Tokyo], Physical Society of Japan, cop. 2014, pp. 013045-1-013045-4.
5. Aleksandra Cvetinović, Jelena Vesić, Andrej Likar, Matej Lipoglavšek, Primož Pelicon, Toni Petrovič, Alberto Sánchez Ortiz, "Electron screening effect in (p,n) and (p,γ) reactions", In: *Seventh European Summer School on Experimental Nuclear Astrophysics, 15-27 September 2013, Santa Tecla, Sicily, Italy*, (AIP conference proceedings, vol. 1595, 2014), New York, American Institute of Physics, 2014, vol. 1595, pp. 238-241, 2014.
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1. Boštjan Črnič, "Izpostavljenost zunanjemu sevanju", In: *Meritve radioaktivnosti v okolju in na izviri ter njihova obravnava v luči morebitnega vpliva NEK na okolje*, Matjaž Korun, et al, 1. izd., Ljubljana, Institut Jožef Stefan, 2014, pp. 79-92.
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1. Toni Petrovič, , P-201300352, Urad RS za intelektualno lastnino, 4.6.2014.
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3. Matjaž Vencelj, Larisa Hosnar, Klemen Bučar, Janez Burger, Angle-sensitive gamma camera with a rotary obstruction, GB1417153.2, Intellectual Property Office, 29.12.2014.

## MENTORING

1. Toni Petrovič, *Algorithms for digital signal processing in radiation detection*: doctoral dissertation, Ljubljana, 2014 (mentor Matej Lipoglavšek; co-mentor Matjaž Vencelj).
2. Rok Bohinc, *X-ray studies of structural and dynamical properties of chlorinated hydrocarbons*: doctoral dissertation, Ljubljana, 2014 (mentor Matjaž Žitnik).
3. Iulija Mikulska, *Structural and magnetic properties of Fe-doped BaTiO<sub>3</sub> ceramics*: doctoral dissertation, Nova Gorica, 2014 (mentor Iztok Arčon; co-mentor Matjaž Valant).
4. Tilen Breclj, : master's thesis, Ljubljana, 2014 (mentor Simon Širca; co-mentor Matej Horvat).
5. Mitja Kelemen, : master's thesis, Ljubljana, 2014 (mentor Primož Pelicon).
6. Boštjan Silič, *Upgrade of the integrating sphere for precise photometric measurements on various light sources*: master's thesis, Nova Gorica, 2014 (mentor Iztok Arčon).
7. Žiga Zaplotnik, : master's thesis, Ljubljana, 2014 (mentor Simon Širca).

# DEPARTMENT OF THIN FILMS AND SURFACES

F-3

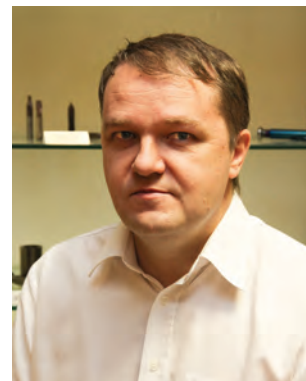
*The main research field of the department is the development, deposition and characterization of hard protective PVD coatings, while research is also conducted in other fields of thin films and surface physics. The basic research is concentrated on studies of the physical and chemical properties of 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.*

In the field of hard protective coatings, the binary (TiN) and ternary coatings (TiAlN) are nowadays predominantly considered as a mature technology. Nevertheless, the research is being performed in several directions in multilayer and composite hard coatings. One of such cases is the blue-colour nanolayer coating AlTiN/TiN, which we patented a few years ago and successfully implemented in industrial production. Though the colour of hard coatings is of minor importance for the tooling industry, it does enable a visual estimate of tool wear, an easier identification of tools, and can act as a recognizable brand for the tool manufacturer. In the past year we published a review paper where we explained the physical background of the colour formation. A good combination of refraction index, absorption coefficient and layer thickness enables the formation of a deep colour, with a minimum dependence of its visual appearance on the observation angle. This was obtained by a precise control of the upper layer thickness (tolerance below 10 nm), with the help of a thin-film growth simulation, which we had previously developed for the industrial deposition chamber CemeCon CC800/9.

In contrast to standard ternary coatings with a 1:1 stoichiometry, we paid a lot of attention to a study of the dependence of the functional properties on the atomic ratio of the two metallic elements. We performed several experiments with the so-called triangular targets of two elements, which enable the deposition of a vertical composition gradient. Using this technique we analysed the systems  $\text{Cr}_x\text{Al}_{1-x}\text{N}$  and  $\text{Cr}_x\text{V}_{1-x}\text{N}$ . If using the classical approach (by monolithic targets) each such analysis would require 20 independent depositions, while in triangular targets only one deposition is sufficient. The application of this method is the topic of our Ph.D student Aljaž Drnovšek, who analysed the samples prepared in this way also from the tribological point of view.

In the field of tribological testing, two more directions of analysis need to be mentioned. The first one is more technologically oriented – the study of adding  $\text{MoS}_2$  nanotubes in synthetic oils, where we study their influence on the lubricating properties for various hard coatings. The second one is oriented on the influence of the surrounding atmosphere (air, oxygen, nitrogen) on tribocorrosion processes for certain coatings. Though this appears to be a simple question, there has been no satisfactory answer in the literature. Yet another analysis from this topic concerns the behaviour at the microlevel, i.e., how do the growth defects evolve during a tribological test. In contrast to standard, long-term tests we performed extremely short tests (only a few movements on the device), and traced the evolution on one particular defect.

The field of growth defects was the topic of the Ph.D of our young researcher dr. Peter Gselman, which he defended at the University of Maribor late last year. He classified the growth defects based on the appearance time (during cleaning, etching or deposition) and based on seed composition (sulphides, simple oxides, mixed oxides). One of the main conclusions was, how much do the various seed types influence subsequent defect growth, which later on defines the coating macroscopic properties (delamination, corrosion resistance). The focused ion beam technique (FIB) was found to be extremely useful for the analysis of individual defects; therefore, we implemented it into a standard analytic procedure for this purpose.



Head:  
**Asst. Prof. Miha Čekada**

**We explained the physical background of the formation of the blue colour in decorative hard coatings AlTiN/TiN.**

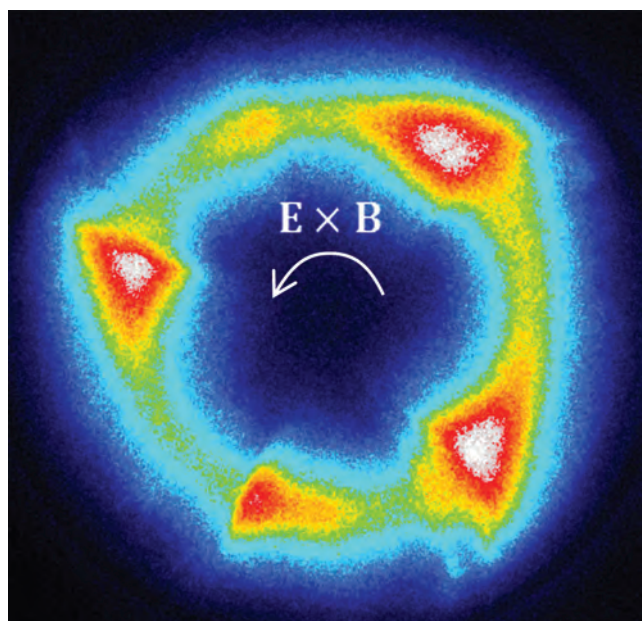


Figure 1: Magnetron plasma, recorded by a high-speed camera (exposure time 10 ns)



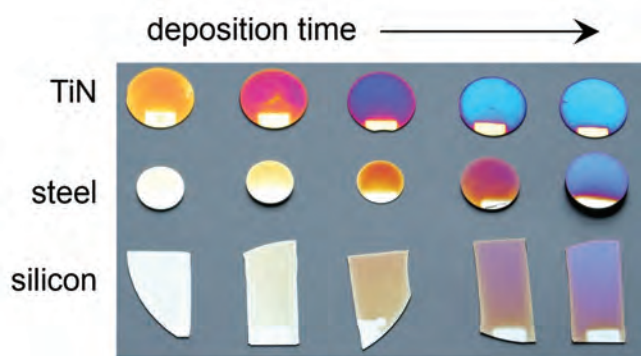


Figure 2: Decorative hard coatings of AlTiN prepared on different substrates at different deposition times of the top layer

The editors of the journal “Plasma Sources Science and Technology” specifically emphasized our paper on ionization zones in magnetron sputtering.

The development of hard coatings is not possible without a deeper knowledge of plasma physics, which is used for the sputtering of thin films. If magnetron plasma is observed with the naked eye or by an ordinary camera, it appears to be symmetrically placed above the cathode (target). However, imaging with a high-speed camera (exposure time below 1  $\mu$ s) reveals that the plasma is not homogeneous; in contrast, periodic structures called the ionization zones appear, and they move in the direction  $E \times B$  with a speed of 5–10 km/s. Dr. Matjaž Panjan and his partners from the Lawrence Berkeley National Laboratory, USA, showed that the ionization zones are a basic feature of magnetron plasma and that they play a decisive role in the transport of charged particles from the cathode to the anode. Measurements using current probes and a mass spectrometer showed that the number and energy of the charged particles (ions and electrons) are symmetrically distributed along the magnetron plane. The asymmetric distribution was explained by the formation of a stable electric field within the rotating ionization zones. The editors of the journal “Plasma Sources Science and Technology” specifically emphasized this paper as a very interesting research work, as published on the journal’s webpage: <http://iopscience.iop.org/0963-0252/labtalk-article/56997>. Dr. Matjaž Panjan presented these results in an invited lecture at the prestigious American Vacuum Society conference in Baltimore, USA.

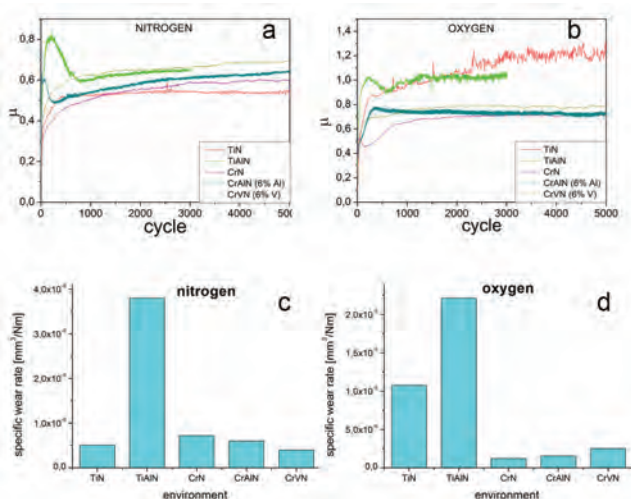


Figure 3: Friction coefficient (a,b) and wear rate (c,d) of different PVD coatings. The tribological tests were performed by a corundum ball in a nitrogen (left) and oxygen atmosphere (right).

To a minor extent, we are engaged in the Eurofusion project, where we are active in two fields. In collaboration with the Max-Planck institute for plasma physics (Garching, Germany) we work on the research of gaseous products in the ASDEX Upgrade tokamak. The second field involves the deposition of tungsten nitride thin films, which was later analysed in fusion reactor conditions by the other project partners. The tungsten nitride spontaneously forms in the reactor inner walls during nitrogen blowing; our sputtered coating is a good approximation of these deposits.

We also work on the possibility of using hard coatings as diffusion barriers against the oxidation of rare-earth magnets (Sm-Co). For this purpose we deposited several coatings on magnets (either bare or nickel-clad) and analysed weight gain at various annealing temperatures.

The majority of our research is at least indirectly connected to industrial applications. In the previous year our main partners were the companies Unior, Kovinos, Phos, Kolektor, EMO Orodjarna, Magneti and Cetis. From the latter company comes our young researcher from the industry Vladan Mladenović. His topic is surface structuring with various machining techniques (scratching, laser treatment, micromilling, electro erosion), and the analysis of these processes at the microlevel using the Taguchi methods of experiment design.

### Some outstanding publications in the past year

1. Panjan, M., Klanjšek Gunde, M., Panjan, P., Čekada, M.: Designing the colour of AlTiN hard coating through interference effect, *Surface & coatings technology*, 254 (2014) 65–72
2. Panjan, M., Franz, R., Anders, A.: Asymmetric particle fluxes from drifting ionization zones in sputtering magnetrons, *Plasma sources science & technology*, 23 (2014) 025007-1–025007-12

### Awards and appointments

1. Peter Gselman: Young researcher award, best oral presentation, Dubrovnik, Croatia, International conference on thin films, “Influence of sulphide and oxide inclusions in steel on growth of TiAlN/CrN nanolayered PVD hard coating”



## INTERNATIONAL PROJECTS

1. Study of Growth Defects in Nanolayer Structures  
Asst. Prof. Miha Čekada  
Slovenian Research Agency
2. Self-organized Plasma Structures in Magnetron Sputtering  
Dr. Matjaž Panjan  
Slovenian Research Agency
3. Plasma Facing Components-1-IPH-FU, EUROFUSION  
Dr. Matjaž Panjan  
European Commission
4. Medium Size Tokamak Campaigns-MST1-FU, EUROFUSION  
Dr. Matjaž Panjan  
European Commission

## RESEARCH PROGRAM

1. Thin Film Structures and Plasma Surface Engineering  
Asst. Prof. Miha Čekada

## R & D GRANTS AND CONTRACTS

1. Organic-Inorganic Thin Film Structures for Electronics Components  
Dr. Peter Panjan
2. Protected Permanent Magnets for Advanced High-Temperature Applications  
Asst. Prof. Miha Čekada
3. Multifunctional Nanostructured Films for Artificial Implants - Corrosion and Tribocorrosion Processes  
Dr. Darinka Kek Merl

4. Research and Development of Rapid Production and Repair in Modern 3D Cutting Tools with Advanced Laser Technologies  
Dr. Peter Panjan
5. Colour, Absorption and Protective Nanolayer Coatings for Aluminium Alloy  
Dr. Peter Panjan
6. Self-lubricating and Wear Resistant PVD Hard Coatings based on (V,Cr,Al,Ti)N for Hot-working Processes  
Dr. Peter Panjan
7. Development and Production of Taylor Made Milling Tools, Coatings and Corresponding Manufacturing Technologies in Individual Tooling Industry  
Asst. Prof. Miha Čekada
8. Functionalization of Biomedical Samples by Thermodynamic NON-equilibrium Gaseous Plasma  
Dr. Peter Panjan
9. Toward Ecologically Benign Alternative for Cleaning of Delicate Biomedical Instruments  
Dr. Peter Panjan
10. Reduction of Friction and Tool Wear using Advanced Lubricants and Protective PVD Coatings  
Dr. Srečko Paskvale

## NEW CONTRACTS

1. Study of Functional Properties of PVD-Hard Coatings in the System (Cr,Al)N  
Dr. Peter Panjan  
Kovinos, d. o. o.
2. Characteristics of Gaseous Plasma in Gaps  
Dr. Peter Panjan  
Kolektor Sikom, d. o. o.

## VISITORS FROM ABROAD

1. Aleksandar Miletić, Pal Terek, University of Novi Sad, Novi Sad, Serbia, 2-7 April 2014
2. Dr. Thomas Schwarz-Selinger, Max-Planck-Institut für Plasmaphysik, Garching, Germany, 2 April 2014
3. Dr. Antti Hakola, VTT Technical Research Centre of Finland, Espoo, Finland, 2 April 2014
4. Dr. André Anders, Lawrence Berkley National Laboratory, Berkley, USA, 3-4 April 2014
5. Suzana Petrović, Vinča nuclear institute, Belgrade, Serbia, 2-6 June 2014
6. Aleksandar Miletić, Pal Terek, University of Novi Sad, Novi Sad, Serbia, 4-5 September 2014
7. Suzana Petrović, Biljana Gaković, Vinča nuclear institute, Belgrade, Serbia, 24-28 November 2014
8. Marko Jerčinović, Ruder Bošković institute, Zagreb, Croatia, 8-10 December 2014
9. Tihomir Car, Ruder Bošković institute, Zagreb, Croatia, 10-12 December 2014

## STAFF

### Researchers

1. Asst. Prof. Miha Čekada, Head
2. Dr. Darinka Kek Merl
3. Dr. Peter Panjan
4. Dr. Matjaž Panjan

### Postdoctoral associate

5. Dr. Srečko Paskvale

### Postgraduates

6. Aljaž Drnovšek, B. Sc.
7. Dr. Peter Gselman, left 01. 11. 14

### Technical and administrative staff

8. Jožko Fišer
9. Damjan Matelič
10. Andrej Mohar
11. Tomaž Sirknik

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### ORIGINAL ARTICLE

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6. Matjaž Finšgar, Darja Kek-Merl, "2-mercaptobenzoxazole as a copper corrosion inhibitor in chloride solution: electrochemistry, 3D-profilometry, and XPS surface analysis", *Corros. sci.*, vol. 80, pp. 82-95, March 2014.

7. Matjaž Finšgar, Darja Kek-Merl, "An electrochemical, long-term immersion, and XPS study of 2-mercaptobenzothiazole as a copper corrosion inhibitor in chloride solution", *Corros. sci.*, vol. 83, pp. 164-175, June 2014.
8. Aleksandar Miletić, Peter Panjan, Branko Škorić, Miha Čekada, Goran Dražić, Janez Kovač, "Microstructure and mechanical properties of nanostructured TiAlSiN coatings deposited by magnetron sputtering", In: Selected papers from the 56th Annual Technical Conference - SVC TechCon of Surface and Coatings Technology, April 20-25, 2013, Providence, Rhode Island, *Surf. coat. technol.*, vol. 241, pp. 105-111, 2014.
9. Matjaž Panjan, Robert Franz, André Anders, "Asymmetric particle fluxes from drifting ionization zones in sputtering magnetrons", *Plasma sources sci. technol.*, vol. 23, no. 2, str- 025007-1-025007-12, 2014.
10. Matjaž Panjan, Marta Klanjšek Gunde, Peter Panjan, Miha Čekada, "Designing the color of AlTiN hard coating through interference effect", *Surf. coat. technol.*, vol. 254, pp. 65-72, 2014.
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12. Mirjana Rodošek, Aleksander Rauter, Lidija Slemenik Perše, Darja Kek-Merl, Angela Šurca Vuk, "Vibrational and corrosion properties of poly(dimethylsiloxane)-based protective coatings for AA 2024 modified with nanosized polyhedral oligomeric silsesquioxane", *Corros. sci.*, vol. 85, pp. 193-203, Aug. 2014.
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2. Aljaž Drnovšek, Peter Panjan, Matjaž Panjan, Srečko Paskvale, Jože Buh, Miha Čekada, "The influence of surrounding atmosphere on tribological properties of hard protective coating", In: *Proceedings*, 57th Annual Technical Conference [of the] Society of the Vacuum Coaters, May 3-8, 2014, Chicago, IL, USA, Albuquerque, Society of Vacuum Coaters, 2014, pp. 311-317.
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## PUBLISHED CONFERENCE CONTRIBUTION

1. Tonica Bončina, Peter Gselman, Darja Kek-Merl, Peter Panjan, Franc Zupanič, "Metallography of hard ceramic coatings", In: *Development and optimization of the castings production processes: proceedings book*, 14th International Foundrymen Conference, Opatija, May 15th-16th, 2014, Faruk Unkić, ed., Sisak, Faculty of Metallurgy, 2014, 7 pp.

## MENTORING

1. Peter Gselman, *PVD-defects and their influence on physicochemical properties of coating/substrate system*: doctoral dissertation, Maribor, 2014 (mentor Franc Zupanič; co-mentor Peter Panjan).

# 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 and ion spectroscopy techniques.*

The surfaces of solid materials are engineered using non-equilibrium gaseous plasma created at low pressures by the appropriate gaseous discharges. Gaseous molecules are partially dissociated and ionized upon inelastic collisions with free electrons. The distribution of neutral as well as charged particles over their kinetic energies is essentially Maxwell-Boltzmann, but electrons have a kinetic temperature between 10,000 and 100,000 K, while other gaseous particles remain close to room temperature. The distribution of molecules over excited states, however, does not follow the Boltzmann law, but can be tailored using appropriate discharge parameters over a broad range over many decades. Such a paradox is explained by the lack of channels for the thermalization of molecules excited to different states. While thermalization is easily achieved at atmospheric pressure, the deviations from this distribution increase with a decreasing pressure. The major reason is the conservation of the total energy and momentum during collisions, which often require three-body events that are unlikely to occur at low pressure. The probability of such collisions increases with the square of the pressure and small deviations from the Boltzmann distribution are already observed at a sub-atmospheric pressure, while at the pressure of 100 Pa the three-body collision frequency becomes as low as  $10 \text{ s}^{-1}$ . Five major paradoxes concerning deviations from thermal equilibrium have been explained in a simplified manner in a monograph published in 2014 by Lampert Academic Publishing. The book, containing about 150 pages, is aimed primarily at users of plasma technologies for the modification of polymers rather than plasma physicists or chemists.

A non-equilibrium plasma created in oxygen is particularly suitable for the oxidation of various solid materials. The chemical reactivity of such a plasma, as compared to oxygen at thermal equilibrium, is just enormous, so the oxidation of any material occurs in a fraction of a second. Polymers are treated essentially at room temperature in order to prevent any modification of their bulk properties. The oxidation of polymer surfaces causes the formation of oxygen-containing functional groups, which is reflected in an improved wettability and thus properties suitable for the rapid adhesion of both inorganic particles and biological cells. The surface modification is monitored by advanced surface-sensitive techniques available in our laboratories, in particular X-ray Photoelectron Spectroscopy (XPS) and Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). A high-resolution carbon 1s XPS spectrum of plasma-treated polystyrene reveals the formation of highly hydrophilic functional groups on the surface of the originally oxygen-free polymer. Such a surface finish of polymer materials makes possible the rapid adhesion and proliferation of biological cells. Not only the substrates, but the cells themselves have been treated with gaseous plasma in order to achieve the desired effects. In such a case a low-pressure environment is unsuitable, so the plasma was created at atmospheric pressure. The biological cells were exposed to a medium that was rich in gold nanoparticles and then treated with gaseous plasma. A high selectivity of the cell destruction was observed, since the benign cells caused apoptosis at a much lower rate than cancer ones.

The textile industry is seeking fabrics of improved functionalities. These products should allow for protection against ultra-violet radiation and should be bacteriostatic. Both effects are achieved by the deposition of nanoparticles onto the textile materials. The adhesion of such nanoparticles, however, is insufficient, so the functionalities vanish



Head:  
**Prof. Miran Mozetič**

**The Scientific Council of the Slovenian Research Agency selected the paper N. Recek at al., Protein Adsorption on Various Plasma-Treated Polyethylene Terephthalate Substrates, Molecules 18 (2013) 12441-12463 as an outstanding achievement and the corresponding author, A. Vesel, presented the achievement at the 9<sup>th</sup> Slovenian Innovation Forum in November 2014.**



*Figure 1: Glowing nitrogen plasma emits radiation at different wavelengths, peaking in the orange part of the optical spectrum*



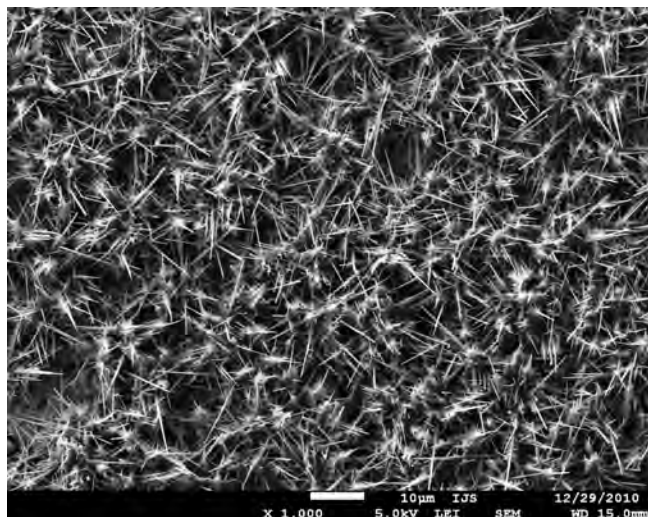


Figure 10: Dense spikes are observed on the SiC surface after treatment with oxygen plasma at 1850 K

after several washing cycles. The reason for poor adhesion is an inadequate surface finish of the fabrics. Systematic research on tailoring the surface properties of cotton fabrics by plasma treatment has been performed. The plasma was generated in different gases. The best results in terms of the adhesion of zinc oxide nanoparticles were achieved using plasma created in moist tetrafluoromethane. The dissociation energy for  $CF_4$  molecules is much higher than for water vapour, so the plasma electrons are likely to form OH and O radicals in such an environment, although the water partial pressure is much lower than the  $CF_4$ . The concentration of F radicals is therefore much lower than OH radicals. Although F radicals bond chemically to the surface of the polymer, the OH and O radicals cause extensive oxidation and the formation of unstable molecular fragments rich in C, H, F and O, which are rapidly desorbed from the surfaces. As a result of such synergistic effects of F- and O-rich radicals substantial etching of the materials, without leaving hydrophobic functional groups on the cellulose fibres, occurs, leading to an optimal surface finish for adhesion of ZnO nanoparticles. Unlike for untreated materials, the ZnO nanoparticles are rather uniformly distributed in the fabrics, which allows for excellent protection against both UV A and B radiation. The amount of ZnO nanoparticles on materials treated under

optimal conditions is double, when compared to the untreated fabrics and the functional properties remain almost unchanged even after several washing cycles.

Textiles are also used as materials for wound dressings. Instead of cotton, which is prohibitively expensive, synthetic cellulose fibres called viscose are used for the dressings. A drawback of the current technologies used for the processing of viscose materials is the suitability for bacteria, which are likely to appear on the wounds.

**Dr. Gregor Primc received the first award for the development of an innovative sensor at the 7<sup>th</sup> International Conference on Technology Transfer.**

The material could be made bactericidal by silver chloride nanoparticles, but such a surface finish would also reduce the proliferation of cells and thus slow down the curing process. The viscose fabrics were treated using plasma created in nitrogen and ammonia in order to functionalize them with nitrogen-containing functional groups that are renowned for their bacteriostatic and weakly bactericidal effects. The treatment effect on the

antimicrobial activity was determined by the AATCC 100-1999 standard test adopted in medicine. The antimicrobial activity of such a surface finish was proven against a couple of Gram-negative bacteria, i.e., *S. aureus* and *E. faecalis*. A 100% reduction of the bacteria was found for *S. aureus*, demonstrating that the nitrogen or ammonia plasma was as efficient as the silver chloride nanoparticles. The efficiency for *E. faecalis* was somehow lower (80% reduction for ammonia-plasma-treated samples versus 100% for silver chloride deposited onto oxygen-plasma-treated samples), but still good compared to current practise. An important advantage of the functionalization using nitrogen or ammonia plasma is the preservation of the excellent wettability of the materials. The contact angle of a water drop on materials functionalized with nitrogen functional groups remained at 30°, while the deposition of the silver chloride nanoparticles caused a substantial loss of hydrophilicity, since the contact angle increased to about 65°. This value is still much better than for untreated viscose materials that exhibit a rather hydrophobic character with a water contact angle of about 90°.

For the textile industry, novel and cost-efficient processes were also developed based on the deposition of polymers with embedded nanoparticles with atmospheric pressure plasma jets. An innovative antibacterial thin film with embedded silver nanoparticles was synthesized through atmospheric pressure plasma discharge and characterized thoroughly. This process was based on the single-step fabrication of nanocomposite films, where silver nanoparticles were fed directly into the discharge zone along with tetramethylsiloxane (TMDSO) and nitrogen as the primary carrier gas. Depending on the discharge parameters, the morphology and stoichiometry of the thin films was tailored. An exceptional 32% of silver nanoparticles were uploaded into the deposited polymer film. The bacterial assays using *E. coli* and *S. aureus* strains showed the effective antibacterial activity of the films and indicate that the fabrication of the nanocomposite films using atmospheric pressure plasma represents a feasible way to overcome the issues related to material surface infections.

Melamine-formaldehyde fibres were synthesized from a meltable pre-polymer of etherified melamine-formaldehyde in the form of a low density fleece, subsequently thermally cured in a conveyor belt oven at temperatures of up to 200 °C and post-heated at 260 °C. A high thermal stability and a small fibre diameter, below 5 µm, made it a serious candidate to be a novel core material for

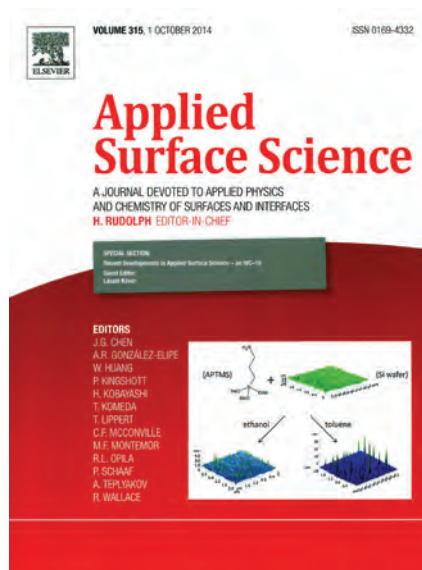


Figure 11: Image on the cover page of Applied Surface Science journal (Vol. 315, 2014) presenting our research on the aminosilane APTMS used for surface modification and adhesion promotion (publication #7)

vacuum thermal insulation panels. The two most crucial core properties, thermal conductivity and outgassing rate, were investigated in thin-walled stainless-steel envelopes, enabling thermal processing combined with a pump-out procedure. A base thermal conductivity of  $\sim 2.3 \text{ mW m}^{-1} \text{ K}^{-1}$  was achieved with randomly oriented fibres at a density of  $\sim 250 \text{ kg m}^{-3}$ . The long-term pressure-rise measurements revealed extremely low outgassing rates,  $q \sim 10^{-15} \text{ mbar L s}^{-1} \text{ cm}^{-2}$ . Additional measurements of the thermal conductivity in a wide pressure range from  $10^{-3} \text{ mbar}$  to atmospheric pressure indicate that these melamine-formaldehyde fibres could be the first organic candidates applied as the core material in vacuum insulating panels with an adequate service lifetime. Their performance is comparable to selected inorganic core materials like glass fibres.

Our group is also involved in the European project IP4Plasma: Industrial innovations based on EU intellectual property assets in the field of atmospheric pressure plasma technology, funded by European Union under the 7th Framework Programme for Research and Innovation. In the IP4Plasma project, plasma-equipment manufacturers and end-users work with leading experts in research to demonstrate the suitability of the atmospheric pressure plasma technology for existing and new industrial applications in the advanced medical diagnostics sector and health-care products. In this project, nine European partners from research and industry areas are involved: Spinverse Ltd (Finland), Fraunhofer Institute for Surface Engineering and Thin Films IST (Germany), IMA (Belgium), Jožef Stefan Institute (Slovenia), LIONEX GmbH (Germany), SOFTAL Corona & Plasma GmbH (Germany), Tosama (Slovenia), VITO - Flemish Institute for Technological Research (Belgium). The IP4Plasma project is scheduled to run for three years between 2014 and 2016. In the frame of the IP4Plasma project a new type of plasma equipment is being developed, capable of the cost- and resource-efficient deposition of coatings, even those containing more complex molecules such as enzymes, on substrates uniformly over full treatment widths of substrates up to 120 cm. The IP4Plasma project also aims to produce new, advanced medical diagnostic products with increased performance and lower cost, including sensitive, quick and cheap tuberculosis and HIV tests and advanced wound-care products with substantially lower production costs and a smaller carbon footprint. Our group is responsible for the precise surface characterization of the plasma-deposited coatings using a new, on-line method to follow the plasma efficiency as well as conventional methods like XPS, ToF-SIMS and AFM.

An alternative method that is suitable for the treatment of delicate materials is the application of a plasma flowing afterglow instead of glowing plasma. Oxygen gas is allowed to pass a discharge region where the plasma is sustained and continues its way to an afterglow chamber. The charged particles neutralize on the way from the discharge region to the afterglow chamber and highly excited metastable atoms quench so the gaseous medium in the afterglow chamber contains only long-living reactive particles, such as neutral atoms in the ground state and molecules in the first electronically excited state. Such particles are reactive enough to interact chemically with materials of high oxidation affinity, but are unlikely to cause substantial etching of other materials such as many types of polymers. The oxygen plasma flowing afterglow was successfully applied for the cleaning of delicate components used in medical practise, such as polymer catheters. The polymer used as the material catheters are made from was deposited onto quartz crystals, contaminated with blood proteins and exposed to both early and late afterglows. The etching rate of the proteins was measured under various conditions rather precisely using a quartz-crystal microbalance. Substantial etching rates of the order of  $\text{nm/s}$  were determined. A rather independent adjustment of the fluxes of neutral atoms and excited molecules allowed for a hypothesis on etching mechanisms. The density of the neutral atoms along the afterglow chamber was determined both theoretically and experimentally and the agreement was almost perfect, showing the reliability of the simulation code. The density of the excited molecules was determined only theoretically due to a lack of reliable experimental methods. The synergistic effects of atoms and excited molecules were found to be crucial for an explanation of the etching rate versus the treatment parameters. The

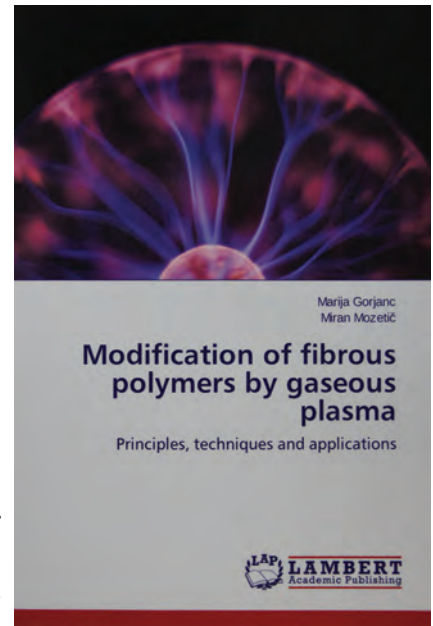


Figure 2: Cover page of the monograph

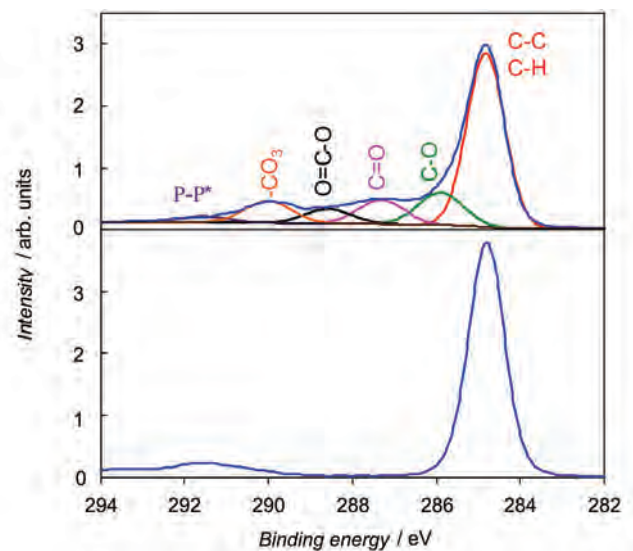


Figure 3: XPS carbon 1s spectra of untreated and oxygen-plasma treated polystyrene

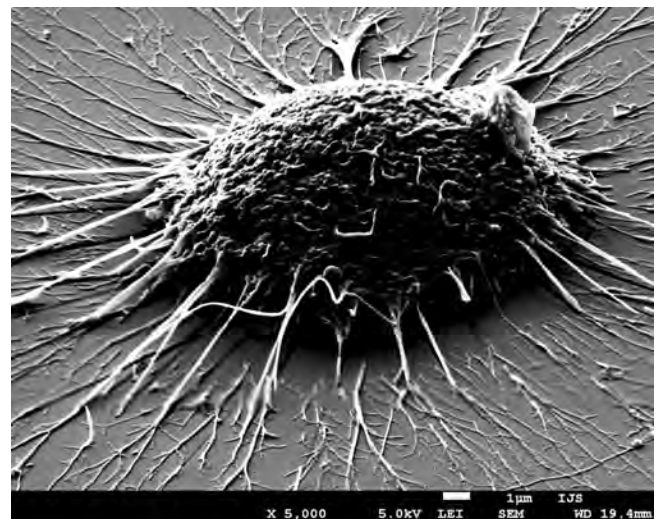


Figure 4: Biological cells feel comfortable on plasma-treated polystyrene



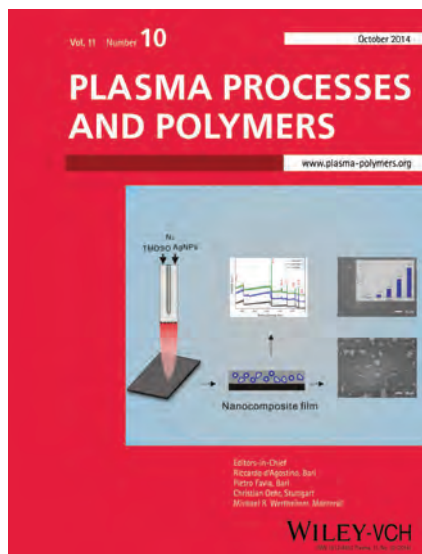


Figure 5: Image from publication #6 appeared on the journal cover page

corresponding scientific paper represents the first report worldwide on such synergistic effects. After removing the blood proteins from the surface of polymer catheters using an oxygen plasma afterglow the substrate surface remains functionalized with polar functional groups. The adsorption kinetics upon the incubation of such materials with blood proteins was studied in details and huge differences between the untreated and cleaned materials were observed. The adsorption kinetics was found to be abnormal for polymers functionalized with polar functional groups, since blood proteins bind to such surfaces both reversibly and irreversibly. Such a kinetic makes the innovative technique useless. The difficulty was successfully overcome by a brief treatment of the cleaned materials for catheters with a fluorine-rich medium that allowed for re-establishing the original surface properties of the treated materials.

Inorganic materials form oxides upon exposure to an oxygen atmosphere at elevated temperature. The oxide is usually in the form of a rather uniform film whose thickness depends on the material properties and the processing temperature. The transformation of oxygen into the plasma state causes substantial differences in the oxidation mechanism. Since the plasma is rich in highly reactive oxygen atoms there is no need for surface dissociation of molecules, so oxidation is achieved at a lower temperature, compared to oxygen at thermal equilibrium. Furthermore, oxygen plasma is rich in fast electrons and slow positive ions so the surface of any material exposed to non-equilibrium gaseous plasma is charged negatively. The charge concentrates at bulges on the surfaces. The electric field between the surface and the substrate is therefore distributed non-uniformly on the surface, so the

electro-migration of metallic ions diffusing through the oxide film onto the surface is favoured towards the peak of a bulge. As a result, the oxide does not grow in the form of a rather uniform thin film, but rather as quasi-one-dimensional structures. The growing mechanism has been elaborated for several types of metal substrates and both the morphological shapes as well as the physiochemical properties of the structures depend on the plasma parameters as well as on the temperatures involved. Since metal oxides are rather poor thermal conductors, strong temperature gradients occur between the peaks of the nanostructures and the bulk material. Such temperature gradients further favour the migration of metallic ions through the oxide nanoparticles, so the nanoparticles form nanowires with a large aspect ratio.

The metal oxides in the form of nanostructures are especially interesting for various applications and the efficient conversion of solar energy in 3<sup>rd</sup> and 4<sup>th</sup> generation of solar cells, photo-catalytic coatings, dye solar cells or water-splitting energy cells. For these applications one needs single crystalline nanowires with the appropriate energy band gap and catalytic activity. There are a number of methods and routes to produce these metal oxide nanowires, but one of the fastest and most efficient is a synthesis by a plasma-assisted

process. A promising material for various applications and especially for water-splitting cells consists of copper oxide nanowires. To achieve efficient performance of water-splitting cells, one needs not only single-crystalline copper oxide nanowire in high densities, but also a homogeneous distribution over large areas on electrodes. This uniform growth of copper oxide nanowires on the top of a copper plate was systematically investigated during

exposure to a radio-frequency oxygen-argon plasma discharge in respect to plasma properties and its localization. An almost uniform growth of nanowires was achieved over a large surface. However, some significant distortions in the nanowire length and shape were found near the edges. Based on experimental results, a theoretical model of nanowire growth was developed, which could predict the maximum lengths of nanowires and the dependence on the plasma parameters. It was demonstrated that the limiting factors for nanowire growth were distortions in the distributions of ions and their local fluxes. In contrast, the heating of materials by the potential interactions of plasma species was found to have little influence on the length of nanowires, and smaller deviations in particle fluxes are allowed for the uniformity of nanowire growth.

The formation of one-dimensional oxide nanoparticles on the surface of silicon carbide samples upon treatment with oxygen-rich gaseous plasma was elaborated. Samples were exposed simultaneously to an oxygen plasma created with a microwave discharge in a resonant cavity and concentrated solar

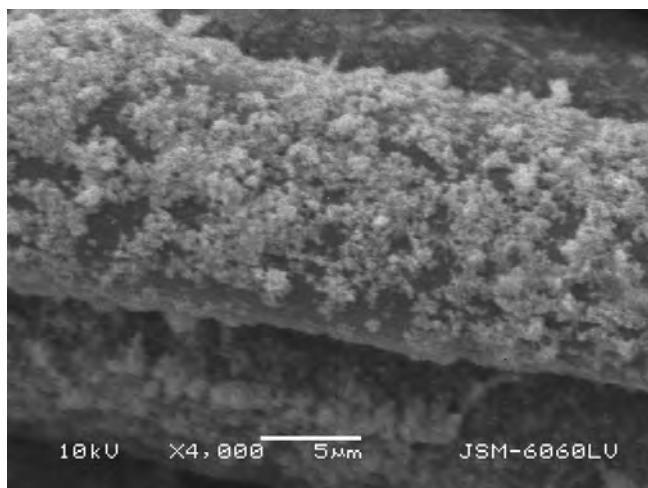


Figure 6: ZnO nanoparticles are dense on plasma-treated cotton

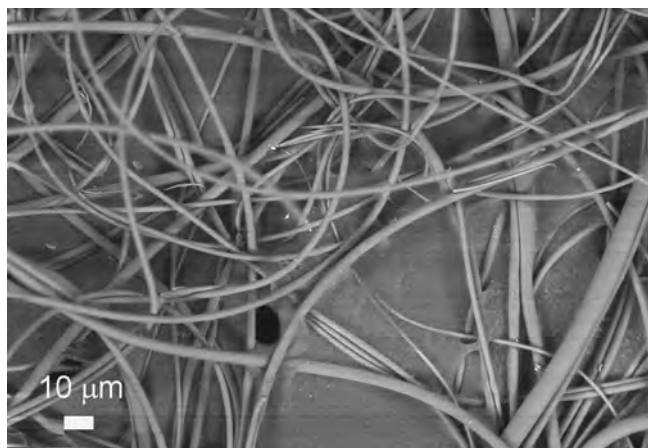


Figure 7: Low-density fleece made from melamine-formaldehyde fibres is suitable for vacuum insulation panels.



radiation. The discharge allowed for a suitable concentration of chemically reactive gaseous particles and free electrons, while the tuneable concentrated solar radiation made it possible to adjust the sample temperature, irrespective of the plasma parameters. A suitable concentration of reactive particles allowed for the excellent chemical reactivity of the gaseous medium, while a large flux of electrons allowed for the appropriate surface charging. The sample temperature was adjusted in the range where the transition from active and passive oxidation is expected at given pressures, i.e., between 1500 and 2000 K. The material remained unchanged up to about 1600 K, but higher temperatures up to about 1900 K caused the growth of nanoparticles. At temperatures above 2000 K all the nanoparticles vanished. The morphology of the nanoparticles depended on the temperature. At the lowest part of the suitable temperature range the nanoparticles grew from nucleation sites unevenly distributed over the sample surface, while elevated temperatures allowed for the synthesizing of dense nano-spikes on the entire surface. The suitable range of temperatures for synthesizing one-dimensional nanoparticles was only about 100 K. The lower-temperature limit was explained by the poor diffusion of Si ions through the oxide, while the upper limit was attributed to active oxidation, causing the removal of such structures.

Aminosilanes are used for surface modification and adhesion promotion. They have the ability to form a durable bond between organic and inorganic materials. A surface modified with aminosilanes has many applications: it can be used in chromatography, as a biosensor in medicine, for attaching metal nanoparticles, and for the detection of specific gases and explosives, etc. In general, it was believed that the aminosilane-modified silicon surface is homogeneous, but this is not always the case. A possible heterogeneity in the surface morphology and the chemistry may be present, and it may significantly influence the application of modified surfaces. Therefore, we investigated the influence of different solvents on the 3-aminopropyltrimethoxysilane (APTMS) modification of Si wafers. In our study we used five solvents with different polarities. We carried out the silanization in a non-polar solvent (toluene), polar aprotic solvents (acetone, N,N-dimethylformamide and acetonitrile) and a polar protic solvent (ethanol) for various deposition times and temperatures. The surface composition, chemical bonding and morphology were characterized by XPS, ToF-SIMS, AFM and SEM methods. Our results show that with the use of the appropriate solvent we can significantly influence the morphology of the modified surface and consequently its adhesion/adsorption properties. Silanization carried out in acetonitrile and toluene leads to the formation of a rough surface with a large density of APTMS polymerized molecules in the form of islands. The surfaces modified in N,N-dimethylformamide were smoother, with a lower density of APTMS islands. When using acetone and ethanol as a solvent we prepared a smooth, thin, modified surface, with a very low density of the APTMS islands.

### Some outstanding publications in the past year

1. Gorjanc, M., Mozetič, M.: Modification of fibrous polymers by gaseous plasma: principles, techniques and applications. Saarbrücken: LAP Lambert Academic Publishing, 2014 Gorjanc, M., Jazbec, K., Šala, M., Zaplotnik, R., Vesel, A., Mozetič, M.: Creating cellulose fibres with excellent UV protective properties using moist CF<sub>4</sub> plasma and ZnO nanoparticles. *Cellulose*, ISSN 0969-0239, 2014, vol. 21, iss. 4, 3007-3021
2. Peršin, Z., Maver, U., Pivec, T., Maver, T., Vesel, A., Mozetič, M., Stana-Kleinschek, K.: Novel cellulose based materials for safe and efficient wound treatment. *Carbohydrate polymers*, ISSN 0144-8617. [Print ed.], jan. 2014, vol. 100, 55-64
3. Cheng, X., Murphy, W., Recek, N., Yan, D., Cvelbar, U., Vesel, A., Mozetič, M., Canady, J., Keidar, M., Sherman, J. H.: Synergistic effect of gold nanoparticles and cold plasma on glioblastoma cancer therapy. *Journal of physics. D, Applied physics*, ISSN 0022-3727, 2014, vol. 47, no. 3, 335402-1-335402-8
4. Vesel, A., Kolar, M., Recek, N., Kutasi, K., Stana-Kleinschek, K., Mozetič, M.: Etching of blood proteins in the early and late flowing afterglow of oxygen plasma. *Plasma processes and polymers*, ISSN 1612-8850, 2014, vol. 11, no. 1, 12-23

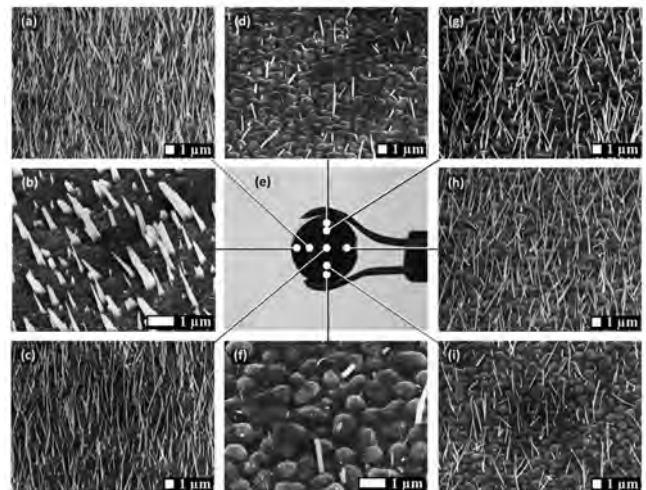


Figure 8: Distortions in the distribution of plasma-synthesized copper oxide nanowires on copper electrodes due to variations in ion fluxes.

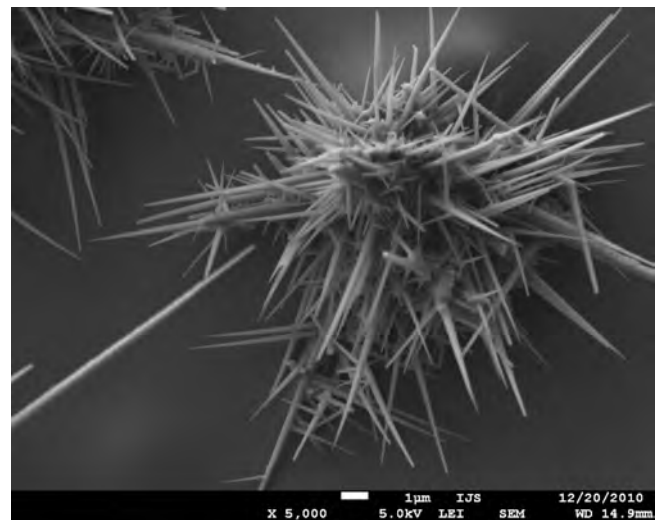


Figure 9: Nano-spikes grow from nucleation sites upon treatment of SiC with oxygen plasma at 1800 K

5. Deng, X., Leys, C., Vujošević, D., Vuksanović, V., Cvelbar, U., De Geyter, N., Morent, R., Nikiforov, A.: Engineering of composite organosilicon thin films with embedded silver nanoparticles via atmospheric pressure plasma process for antibacterial activity. *Plasma processes and polymers*, ISSN 1612-8850, 2014, vol. 11, no. 10, 921-930
6. Jakša, G., Štefane, B., Kovač, J.: Influence of different solvents on the morphology of APTMS-modified silicon surfaces. *Applied Surface Science*, ISSN 0169-4332. [Print ed.], 2014, vol. 315, no. 1, 516-522
7. Jovanović, Z., Spreitzer, M., Kovač, J., Klement, D., Suvorov, D.: Silicon surface deoxidation using strontium oxide deposited with the pulsed laser deposition technique. *ACS applied materials & interfaces*, ISSN 1944-8244. [Print ed.], 2014, vol. 6, issue 20, 18205-18214

## Awards and appointments

1. Dr. Gregor Primc: 1st award for innovation "Laser Fiber Optic Catalytic sensor". The award was given at 7th International Technology Transfer Conference

## Organization of conferences, congresses and meetings

1. 9th EU-Japan Joint Symposium on Plasma Processing (JSPP2014) and EU COST MP1101 Workshop on Atmospheric Plasma Processes and Sources, Bohinjška Bistrica, 19–23 January 2014
2. COST Action: TD1208: Training School Title: Chemistry initiated by electrical discharges with liquids, Ljubljana, 3–6 February 2014

## Patent granted

1. Ita Junkar, Miran Mozetič, Alenka Vesel, Uroš Cvelbar, Metka Krašna, Dragoslav Domanovič, Method of treatment of biomedical polymeric prosthesis for improvement of their antithrombogenic properties, AT513072 (B1), Österreichisches Patentamt, 15.2.2014.

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## INTERNATIONAL PROJECTS

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. EFDA-JET 2013 Experimental Campaigns<br/>Dr. Aleksander Drenik<br/>Ministry of Education, Science and Sport</li> <li>2. EFDA-JET 2013 Analysis of Mixed Materials on ITER-like Wall Samples Using XPS/AES<br/>Dr. Vincenc Nemanič<br/>Ministry of Education, Science and Sport</li> <li>3. 7FP - IP4Plasma; Industrial Innovations Based on EU Intellectual Property Assets in the Field of Atmospheric Plasma Technology<br/>Asst. Prof. Janez Kovač<br/>European Commission</li> <li>4. COST MP1101; Biomedical Applications of Atmospheric Pressure Plasma Technology<br/>Prof. Uroš Cvelbar<br/>COST Office</li> <li>5. COST TD1208; Electrical Discharges with Liquids for Future Applications; COST Training School on Liquid Discharges<br/>Prof. Uroš Cvelbar<br/>COST Office</li> <li>6. NATO Grant; SPS 984555; Atmospheric Pressure Plasma Jet for Neutralisation of CBW<br/>Prof. Uroš Cvelbar<br/>Nato - North Atlantic Treaty Organisation</li> <li>7. Development and Investigation of Optimal Regimes of RF Conditioning of Uranan-2M Vacuum Chamber Walls using Optical and Probe Methods of Plasma Diagnostics<br/>Prof. Miran Mozetič<br/>Slovenian Research Agency</li> <li>8. Characterization of Non-equilibrium Plasma for Modification of Nano and Biocompatible Materials<br/>Prof. Miran Mozetič<br/>Slovenian Research Agency</li> <li>9. Ultra Nanoporous Nanowires of Metal Oxides<br/>Prof. Uroš Cvelbar<br/>Slovenian Research Agency</li> <li>10. Characterization of Processing Plasma with Catalytic and Cutoff Probes<br/>Prof. Miran Mozetič<br/>Slovenian Research Agency</li> <li>11. Advanced Physical Techniques for Modification of Polymer and Composite Functionalities for Biomedical Applications<br/>Prof. Miran Mozetič<br/>Slovenian Research Agency</li> <li>12. Guided Nanoherding of Quantum Dots</li> </ol> | <ol style="list-style-type: none"> <li>Prof. Uroš Cvelbar<br/>Slovenian Research Agency</li> <li>13. Molecular Imaging of Biological Samples Using MeV Ions and keV Clusters for TOF-SIMS Spectrometry<br/>Asst. Prof. Janez Kovač<br/>Slovenian Research Agency</li> <li>14. Deposition of Coatings on Plasma Prepared Medical Stents<br/>Prof. Uroš Cvelbar<br/>Slovenian Research Agency</li> <li>15. Synthesis and Characterization of Pt Nanocatalysts at Metal Oxide based Supports for Fuel Cells Application<br/>Asst. Prof. Alenka Vesel<br/>Slovenian Research Agency</li> <li>16. Ion and Laser Beam induced Formation of Biocompatible Alloys in Multilayered Thin Film Structures<br/>Asst. Prof. Janez Kovač<br/>Slovenian Research Agency</li> <li>17. Measurements of Plasma Parameters in Capacitive and Inductive RF Discharges<br/>Prof. Uroš Cvelbar<br/>Slovenian Research Agency</li> <li>18. Characterization of Gaseous Plasma for Nanoparticle Synthesis<br/>Asst. Prof. Alenka Vesel<br/>Slovenian Research Agency</li> <li>19. ECS Electrochemical Society<br/>Prof. Uroš Cvelbar<br/>Slovenian Research Agency</li> <li>20. Plasma Facing Components-I-IPH-FU, EUROFUSION<br/>Dr. Aleksander Drenik<br/>European Commission</li> <li>21. Education-ED-FU, EUROFUSION<br/>Prof. Miran Mozetič<br/>European Commission</li> <li>22. JET Campaigns-JET1-FU, EUROFUSION<br/>Dr. Aleksander Drenik<br/>European Commission</li> <li>23. Medium Size Tokamak Campaigns-MST1-FU, EUROFUSION<br/>Dr. Aleksander Drenik<br/>European Commission</li> </ol> |
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## RESEARCH PROGRAMS

1. Vacuum Technique and Materials for Electronics  
Dr. Vincenc Nemanič
2. Thin Film Structures and Plasma Surface Engineering  
Prof. Miran Mozetič

## R & D GRANTS AND CONTRACTS

1. Organic-Inorganic Thin Film Structures for Electronics Components  
Asst. Prof. Janez Kovač
2. Development of Advanced Processes for Attending High Efficient Nano Modified Textile Materials  
Prof. Miran Mozetič
3. Multifunctional Nanostructured Films for Artificial Implants - Corrosion and Tribo-corrosion Processes  
Asst. Prof. Janez Kovač
4. Synthesis of Nanowires for Regenerative Energy Cells  
Prof. Uroš Cvelbar
5. Colour, Absorption and Protective Nanolayer Coatings for Aluminium Alloy  
Asst. Prof. Janez Kovač
6. Self-lubricating and Wear Resistant PVD Hard Coatings based on (V,Cr,Al,Ti)N for Hot-working Processes  
Dr. Peter Panjan
7. Development of the Functional Textiles used for the Treatment of Diabetic Foot (Malum perforans)  
Prof. Miran Mozetič
8. New Materials for Printed Sensors and Indicators and their Integration in Smart Printed Matter  
Asst. Prof. Alenka Vesel
9. Interaction between Fully Dissociated Moderately Ionized Ammonia Plasma and Glass-

- fiber Reinforced Polymers  
Prof. Miran Mozetič
10. Nanostructures and Related Composites for Detection of Hazardous Gaseous Molecules  
Prof. Uroš Cvelbar
  11. Functionalization of Biomedical Samples by Thermodynamic Non-equilibrium Gaseous Plasma  
Prof. Miran Mozetič
  12. Toward Ecologically Benign Alternative for Cleaning of Delicate Biomedical Instruments  
Asst. Prof. Alenka Vesel
  13. Functionalization of Polymer Cardiovascular Implants for Optimal Hemocompatibility  
Asst. Prof. Alenka Vesel

## NEW CONTRACTS

1. Advanced Functional Implant  
Dr. Ita Junkar  
Ekliptik, d. o. o.
2. Environmentally Friendly Cleaning of Components for Large Vacuum Systems  
Prof. Miran Mozetič  
Vacutech Vacuum Technologies and Systems, d. o. o.
3. Characteristics of Gaseous Plasma in Gaps  
Prof. Uroš Cvelbar  
Kolektor Sikom, d. o. o.
4. Investigation of Evaluation Methods for Vacuum Insulation Panel Performance Testing in Accordance with Draft of ISO Standard  
Dr. Vincenc Nemanič  
Stirolab, d. o. o.
5. Investigation of Melamine Foams as the Core Material in Vacuum Thermal Insulation  
Dr. Vincenc Nemanič  
Melamin Chemical Factory, d. d.

## VISITORS FROM ABROAD

1. Dr. Thomas Gries, University of Lorraine, Lorraine, France, 23–25 January 2014
2. Prof. Tara Desai, IAEA, Wien, Austria, 16–18 March 2014
3. Dr. Andre Anders, Lawrence Berkley National Laboratory, Berkley, USA, 3–6 April 2014
4. Dr. Oleh Baranov, Kharkov Aviation Institute, Kharkov, Ukraine, 15–31 May 2014
5. Prof. Ho-Sung Yoon, Kyungpook University, Daegu, South Korea, 29–31 May 2014
6. Prof. Thomas Sabu, Mahatma Ghandi University, Kerala, India, 2–4 June 2014
7. Dr. Joanna Izdebska, University of Warsaw, Warsaw, Poland, 2–4 June 2014
8. Dr. Davor Peruško, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 1–6 June 2014
9. Dr. Suzana Petrović, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 1–6 June 2014
10. Prof. Hong Young Chang, KAIST, Daejeon, South Korea, 20–26 June 2014
11. Dr. Byung Kuen Na, KAIST, Daejeon, South Korea, 20–26 June 2014
12. Dr. Rachmat Wibowo, Primož Eiselt and Heinz Schmidt, Plasmait GmbH, Lebring, Austria, 24 June 2014
13. Dr. Petr Slobodian, Tomas Bata University, Zlin, Czech Republic, 21–27 July 2014
14. Dr. Yumiko Akanuma, Nissan Motor Co., Ltd., Kanagawa, Japan, 22–24 September 2014
15. Prof. Val Vullev, University of California, California, USA, 17–19 October 2014
16. Akhil Chandran Mukkattu Kuniyil, University of Novi Sad, Novi Sad, Serbia, 7–28 October 2014
17. Dr. Jorge Andres Lopez Garcia, Tomas Bata University, Zlin, Czech Republic, 1 September–31 October 2014
18. Dr. Danijela Vujošević, Institute for Public Health of Montenegro, Podgorica, Montenegro, 6–9 November 2014
19. Dr. Marko Karlušić, Ruder Bošković Institute, Zagreb, Croatia, 20–21 November 2014
20. Dr. Danijela Vujošević, Institute for Public Health of Montenegro, Podgorica, Montenegro, 17–22 December 2014

## STAFF

### Researchers

1. Prof. Uroš Cvelbar
2. Dr. Aleksander Drenik
3. Dr. Ita Junkar
4. Asst. Prof. Janez Kovač
5. Prof. Miran Mozetič, Head
6. Dr. Vincenc Nemanič
7. Asst. Prof. Alenka Vesel

### Postdoctoral associates

8. Dr. Kristina Eleršič, *left 01. 04. 14*
9. Dr. Martina Modic
10. Dr. Gregor Primc
11. Dr. Rok Zaplotnik

### Postgraduates

12. Gregor Filipič, B. Sc.
13. Nataša Hojnik, B. Sc.
14. Gregor Jakša, B. Sc.
15. Nina Recek, B. Sc.
16. Matic Resnik, B. Sc.

### Technical officer

17. Tatjana Filipič, B. Sc.
18. Marko Žumer, B. Sc.

### Technical and administrative staff

19. Urška Kisovec, B. Sc.
20. Janez Trtnik



# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. A. Altaaweel, Gregor Filipič, T. Gries, Thierry Belmonte, "Controlled growth of copper oxide nanostructures by atmospheric pressure micro-afterglow", *J. Cryst. Growth*, vol. 407, pp. 17-24, 2014.
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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.*



Head:

**Prof. Igor Muševič**

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  $T_1$  via field cycling,
- Nuclear double resonance and quadrupole double resonance such as  $^{17}\text{O}$ -H and  $^{14}\text{N}$ -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  $10^2$  Hz to  $10^9$  Hz,
- Electron microscopy and scanning tunnelling microscopy,
- Atomic force microscopy and force spectroscopy,
- Dynamic specific heat measurements.

The research program of the Department of Solid State Physics at the “Jožef Stefan Institute” is performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the Jožef Stefan International Postgraduate School. In 2013, 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

## ***1. 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 a study of physical phenomena in condensed matter at the atomic and molecular levels. The purpose of the investigations was to discover the basic laws of physics governing the behaviour of the investigated systems. The obtained knowledge provides the key to the understanding of microscopic and mac-

**The group has discovered the first superconducting, high-entropy alloy, quantum magnetism in low-dimensional spin systems, physical properties of nanostructures, materials with giant electrocaloric and thermomechanical effects, and multiferroic and relaxor phases. The research included pharmaceutical and biological substances, where an NQR-based portable sensor for distinguishing bring original and forged drugs was developed.**

roscopic properties of various types of solids and is an important condition for the discovery and development of new multifunctional materials and nanomaterials for novel technological applications.

In our research, we used the following experimental techniques:

- Nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) and nuclear quadrupole resonance (NQR),
- Nuclear double resonance  $^{17}\text{O}$ -H and  $^{14}\text{N}$ -H,
- Fast field cycling NMR relaxometry,
- Linear and non-linear dielectric spectroscopy in the range  $10^2$  Hz to  $10^9$  Hz,
- Frequency-dependent ac calorimetry,
- Measurement of electrical and thermal transport coefficients,
- Magnetic measurements.

The research program was performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics, and the Jožef Stefan International Postgraduate School. The investigations were focused on the following research fields:

### Discovery of a superconducting high-entropy alloy

Traditionally, metallic alloy systems have been based mainly on one principal chemical element as the matrix, even though a substantial number of other elements were incorporated for property/processing enhancement.

Within the past several years, a new approach to metallic alloy design with multiple principal elements in equimolar or near-equimolar ratios, termed high-entropy alloys (HEAs), has been proposed. According to this concept, the high entropy of mixing can stabilize disordered solid-solution phases with simple structures like a body-centred cubic (bcc) or a face-centred cubic (fcc) with small unit cells, in competition with ordered crystalline intermetallic phases that often contain structurally complex giant unit cells. The HEA structure is characterized by a topologically ordered lattice with an exceedingly high chemical (substitutional) disorder, so that a HEA can be conveniently termed as a “*metallic glass on an ordered lattice*”. The physical properties of HEAs remain largely unexplored. In 2014, the group of prof. Janez Dolinšek discovered the first superconducting HEA within the Ta-Nb-Hf-Zr-Ti system (Koželj *et al.* Phys. Rev. Lett. 113, 107001 (2014)), showing a high superconducting transition temperature (for a metallic system) of 7.3 K and a large upper critical field of 8.2 T. The temperature-dependent electrical resistivity of the Ta-Nb-Hf-Zr-Ti HEA is shown in Fig. 1.

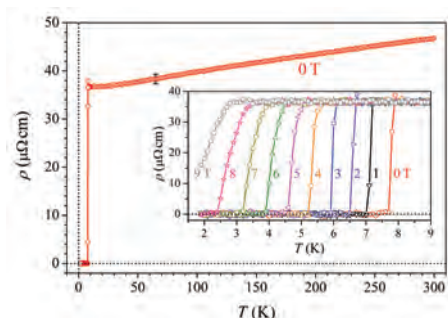


Figure 1: Electrical resistivity of a Ta-Nb-Hf-Zr-Ti high-entropy alloy in the region of the phase transition to the superconducting state.

### Quantum magnetism

Andrej Zorko, Denis Arčon and collaborators discovered the first realization of phase separation in a pure spin system. Phase separation breaking the translational symmetry of a Hamiltonian on a local scale is particularly intriguing, as it regularly appears in chemically homogeneous systems and is related to some fundamental functional properties of materials, such as the colossal magnetoresistance of manganites, the giant electrostriction of relaxors, and possibly even high- $T_c$  superconductivity. The conventional paradigm where electronic charge plays the leading role in promoting phase-separated states when competing phases are present in the solid state has been proven wrong in the case of  $\alpha$ - $\text{NaMnO}_2$ . Here, a novel kind of a phase-separated state was identified and suggested to be due to the interplay of geometrical frustration and a structural instability of the lattice, leading to a magnetostructural inhomogeneity at the nanoscale. The results were published in the paper A. Zorko *et al.*, “Frustration-induced nanometre-scale inhomogeneity in a triangular antiferromagnet”, Nat. Commun. 5, 3222 (2014).

Andrej Zorko and collaborators investigated spin dynamics and disorder effects in a spin-liquid phase of the quantum antiferromagnetic known as the mineral kapellasite. The authors have found that despite a variety of magnetic environments due to a severe random depletion of the magnetic kagome lattice by 27%, the system remains homogeneous with a unique spin susceptibility at high temperatures. Moreover, in the low-temperature, correlated, spin-liquid regime, a broad distribution of spin-lattice NMR relaxation times was observed and ascribed to the presence of local low-energy modes. The findings were published in the paper E. Kermarrec *et al.*, “Spin dynamics and disorder effects in the  $S = 1/2$  kagome Heisenberg spin-liquid phase of kapellasite”, Phys. Rev. B, 90, 205103 (2014).

Martin Klanjšek was invited by the editors of the Physics journal to write a review paper about quantum criticality in spin systems. The journal publishes review papers about the works

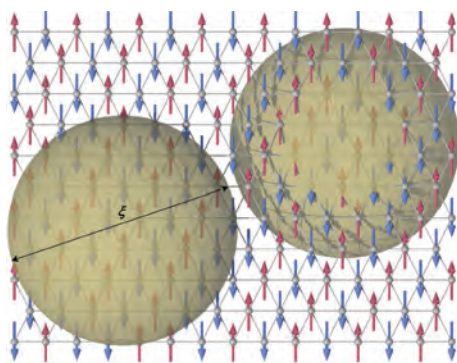


Figure 2: Illustration of the magnetostructurally inhomogeneous ground state of  $\alpha$ - $\text{NaMnO}_2$ , with the monoclinic antiferromagnetic phase being randomly disturbed by defect triclinic regions (spheres).

published in Phys. Rev. Lett. and Phys. Rev. X. In the paper, he generally described an interesting and topical phenomenon of quantum criticality (Figure 3), which leads to the most complicated currently known quantum states in nature. To understand them, it is worth studying the systems with a few degrees of freedom, like one-dimensional quantum spin systems. The paper describes a recent interesting NMR experiment on  $\text{CoNb}_2\text{O}_6$ , which is a realization of the transverse field Ising ferromagnet. This is the simplest quantum-mechanical many-body model featuring even the analytical predictions, fully confirmed by the experiment for the first time. The results are placed in the context of other recent works on quantum criticality, where the author also took part. The paper was published in M. Klanjšek, "A Critical Test of Quantum Criticality", Physics 7, 74 (2014).

#### Diluted magnetic oxides

Andrej Zorko, Denis Arčon and collaborators addressed the pending question of the intrinsic/extrinsic nature of the Mn-induced magnetism of the wide-band-gap perovskite  $\text{SrTiO}_3$ . They showed that this diluted magnetic oxide remains paramagnetic down to low temperatures, in contrast to previous suggestions of intrinsic magnetic freezing. Moreover, using local-probe magnetic-characterization techniques of muon spin relaxation and electron spin resonance they demonstrated that the dopants partially aggregate into nanosized clusters. Their findings were published in the paper A. Zorko *et al.*, "Intrinsic paramagnetism and aggregation of manganese dopants in  $\text{SrTiO}_3$ ", Phys. Rev. B, 89, 094418 (2014).

#### Unconventional molecular superconductors

Anton Potočnik, Peter Jeglič, Denis Arčon and collaborators from the UK, Estonia and Japan studied unconventional superconductivity in expanded fullerides and rare-earth carbides. First they reported a nuclear magnetic resonance (NMR) study of face-centred-cubic  $\text{Cs}_3\text{C}_{60}$ , which can be tuned continuously through the insulator-to-metal transition by pressure. For large interfullerene separations they observed a large non-BCS but s-wave gap in a superconductor, which upon further pressurization approaches the weak-coupling BCS value (Figure 4). These results indicate the importance of the electronic correlations for the pairing interaction and were published in the paper A. Potočnik *et al.*, "Size and symmetry of the superconducting gap in the f.c.c.  $\text{Cs}_3\text{C}_{60}$  polymorph close to the metal-Mott insulator boundary", Sci. Rep. 4, 4265 (2014).

In their second study they observed the freezing of the dynamic Jahn-Teller effect in the Mott insulating state of the metrically cubic but merohedrally disordered  $\text{Cs}_3\text{C}_{60}$  by low-temperature magic-angle spinning NMR. These results were published in the paper A. Potočnik *et al.*, "Jahn-Teller orbital glass state in the expanded fcc  $\text{Cs}_3\text{C}_{60}$  fulleride", Chem. Sci. 5, 3008 (2014). Finally, they investigated the rare-earth carbide,  $\text{La}_2\text{C}_3$ , which showed abnormal behaviour that dramatically deviated from the conventional s-wave superconductors. Such an unconventional response in the local static and dynamic spin susceptibilities was discussed in terms of a possible mixture of spin-singlet and spin-triplet Cooper pairs, which may be promoted by the asymmetric spin-orbit coupling in the system without the centre of inversion. Their findings were published in the paper A. Potočnik *et al.*, "Anomalous local spin susceptibilities in noncentrosymmetric  $\text{La}_2\text{C}_3$  superconductor", Phys. Rev. B 90, 104507 (2014).

#### Cocrystals

Cocrystals are often used in crystal engineering. A cocrystal is a nonionic supramolecular complex that is constructed through several types of interaction, including hydrogen bonding and van der Waals forces.  $^{14}\text{N}$  NQR represents a very sensitive tool for the study of crystal structure and intermolecular interactions in hydrogen bonded cocrystals. Cocrystals of 2,3,5,6-tetramethylpyrazine and several carboxylic acids have been studied with complete  $^{14}\text{N}$  NQR. The  $^{14}\text{N}$  nuclear quadrupole resonance spectra have been used to check whether the cocrystals are indeed formed and to investigate the hydrogen-bonding scheme of 2,3,5,6-tetramethylpyrazine molecules. Published in J. Seliger *et al.*, J. Phys. Chem. B 118, 996–1002 (2014), J. Seliger, V. Žagar, Phys. Chem. Chem. Phys. 16, 18141–18147 (2014).

#### Pharmaceutical substances

$^{14}\text{N}$  NQR represents a useful tool to characterize pharmaceutical substances and the method of their preparation. In combination with a quantum chemical calculation the electron structure of these molecules and the properties of functional groups can be determined.  $^{14}\text{N}$  nuclear quad-

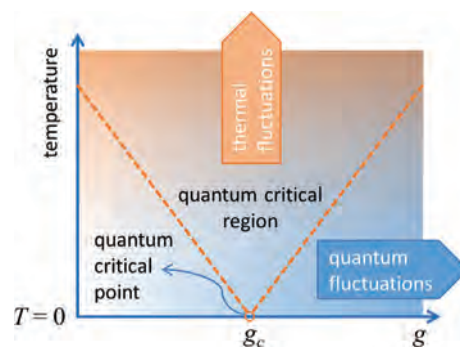


Figure 3: Quantum fluctuations controlled by the non-thermal parameter  $g$  lead to the phase transition at a critical value  $g_c$ , the so-called quantum-critical point, already at zero temperature,  $T = 0$ . Their interplay with thermal fluctuations opens up a characteristic V-shaped quantum-critical region.

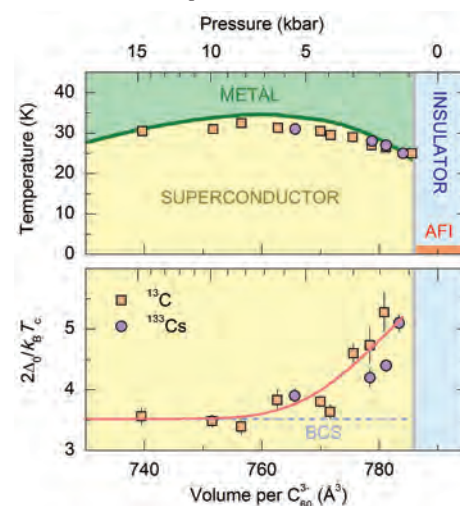


Figure 4: The low-temperature phase diagram and the superconducting gap of face-centred-cubic  $\text{Cs}_3\text{C}_{60}$  as derived from the NMR measurements in the superconducting state.

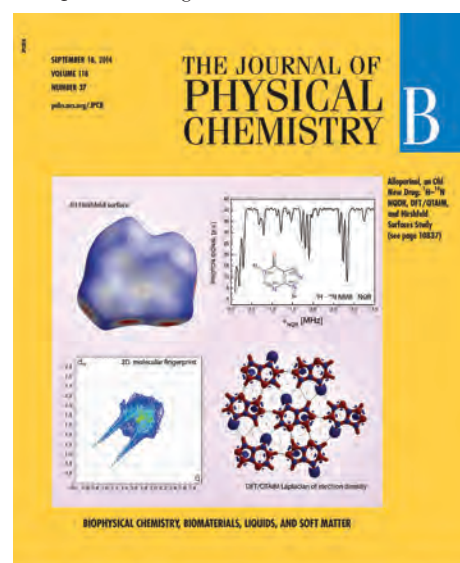


Figure 5: The figure from our paper J. N. Latosinska, *et al.*, was selected for the cover of J. Phys. Chem. B.



rupole resonance (NQR) in two known polymorphs of famotidine was measured. At room temperature, seven quadrupolar sets of transition frequencies corresponding to seven different nitrogen sites in the crystal structure of each of the two polymorphs were found. The NQR frequencies, line shapes, and tentative assignation to all seven molecular  $^{14}\text{N}$  atoms were obtained. Published in J. Lužnik, et al., J. Pharm. Sci. 103, 2704-2709 (2014). Allopurinol (1,5-dihydro-4H-pyrazolo [3,4-d]pyrimidin-4-one), is an active pharmaceutical ingredient of the drugs, applied for the treatment of gout and tumour lysis syndrome. It was recently discovered to have multifaceted therapeutic potential, and hypoxanthine, which is a naturally occurring purine, has been studied experimentally in the solid state by  $^1\text{H}$ – $^{14}\text{N}$  NMR-NQR double resonance by J. N. Latosinska, et al., J. Phys. Chem. B 118, 10837–10853 (2014). This study demonstrated the advantages of combining NQR, DFT/QTAIM, and Hirshfeld surface analysis to extract detailed information on electron density distribution and complex H-bonding networks in crystals of purinic type heterocycles, relevant in pharmacological processes. Figure 5 shows cover of J. Phys. Chem. B featuring a figure from our paper in this number.

Three anhydrous methylxanthines, i.e., caffeine, theophylline and theobromine, have been studied by the same group experimentally in solid state by  $^1\text{H}$ – $^{14}\text{N}$  NMR-NQR (nuclear magnetic resonance–nuclear quadrupole resonance) double resonance (NQDR). Published in J. N. Latosinska, et al., J. Chem. Inf. Model. 54, 2570–2584 (2014).

### Liquid crystals

In a paper A. Gradišek et al., J. Phys. Chem. B 118, 5600–5607 (2014), a detailed study of the cross-relaxation effects between the  $^1\text{H}$  and  $^2\text{H}$  spin systems is presented in the nematic phase of a 5-cyanobiphenyl (5CB) liquid crystal, partially deuterated at  $\alpha$  position (5CB- $\alpha\text{d}2$ ). In the low-frequency domain, the spin–lattice relaxation rate ( $T_1^{-1}$ ) dispersion clearly differs from that of the fully protonated 5CB homologue, as it shows two local maxima at distinct frequencies,  $T_1^{-1}$  presents two distinct local maxima and for low frequencies  $T_1^{-1}$  presents stronger frequency dependence when compared with what is observed for 5CB. The  $T_1^{-1}$  dispersion obtained for 5CB- $\alpha\text{d}2$  for frequencies above 60 kHz was interpreted in terms of the relaxation mechanisms usually accepted to interpret the spin–lattice relaxation in nematic phases in general and 5CB in particular. For lower frequencies it was necessary to consider cross-relaxation contributions between the proton and deuterium reservoirs. The analysis of the quadrupolar relaxation independently confirms that the order director fluctuations are the dominant mechanism of proton relaxation in the low-frequency domain.

### Counterfeit pharmaceuticals interception using nuclear quadrupole resonance

In cooperation with the EU project CONPHIRMER partners from King's College London, Franco-German Research Institute St. Louis, Institute of Mathematics, Physics and Mechanics, Post-graduate School of the J. Stefan Institute, Lund University, industrial partners, and end-users, we have developed a prototype of a medicines authentication device. A prototype portable N-14 nuclear quadrupole resonance based easy-to-use device was developed, which made it possible to distinguish an original and a forged drug. The advantage of the method is that during the scan medicines can remain in original, unopened package and can be later used as intended. The prototype of the device was successfully tested at the end user's location – at the post customs service at Warsaw airport.

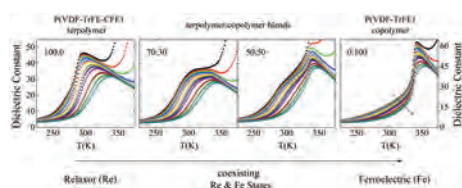


Figure 6: Blending a relaxor terpolymer with a ferroelectric copolymer resulted in a system with coexisting ferroelectric and relaxor states, thus our polymer-blend approach could be suggested as a model method for tailoring various properties of relaxor polymers.

### Relaxor ferroelectrics

Investigations of electroactive polymers have so far mainly focused on either normal ferroelectric polymers or systems that are completely transformed into a relaxor. Only recently properties of the P(VDF-TrFE) copolymer, irradiated with low doses of high-energy electrons, have been reported. Clear evidence that ferroelectric and relaxor states coexist has been provided and it has furthermore been shown that such a coexistence strongly influences various material properties. Since irradiation also creates undesirable side effects, we have, in collaboration with researchers from Pennsylvania State University, developed a polymer system where a similar coexistence of states could be expected: blends of relaxor P(VDF-TrFE-CFE) terpolymer and ferroelectric P(VDF-TrFE) copolymer. We showed that blends entirely exhibit a relaxor dielectric response at a low copolymer content, while in samples with 20-50 wt. % of P(VDF-TrFE) the ferroelectric and relaxor states coexist. DSC data clearly revealed that both components form separate crystalline phases and also the influence of blending on the crystallinity and melting points of both components. Moreover, the relative crystallinity data, obtained from the normalized enthalpy changes at melting, excellently explain the variation of the dielectric constant in developed blends. Published in Casar et al., J. Appl. Phys. 115, 104101 (2014).

### Liquid-crystalline elastomers

A new series of composite liquid-crystalline elastomers was developed, containing both nematogenic and smectogenic molecules. By varying the ratio of the two mesogen species, the width of the temperature interval of the nematic phase, intermediate between the high temperature isotropic and the low temperature smectic A phase, can be controlled. A temperature-concentration phase diagram of this system has been determined via DSC and X-ray diffraction, as well as independently via stress vs. strain measurements. These indicate a possible re-entrant nematic phase for higher values of the mechanical load. Moreover, a soft-elasticitylike behaviour has been detected at low temperatures for systems in the vicinity of the characteristic concentration of the nematogen, below which the nematic phase vanishes.

Published in Domenici et al., RSC Advances 4, 44056-44064 (2014).

### Nanomaterials

An *in-situ* doping approach was successfully employed for the synthesis of  $Mn^{2+}$ -doped sodium titanate nanoribbons, which were used as a precursor for the preparation of  $TiO_2$  nanoribbons with a homogenous distribution of  $Mn^{2+}$  ions. The comprehensive structural characterization using powder X-ray diffraction and electron paramagnetic resonance provided evidence that the  $Mn^{2+}$  ion predominantly substitutes for the  $Ti^{4+}$  ion at octahedral coordination sites in a bulk. Measurements performed on individual nanoribbons using near-edge X-ray absorption fine structure spectromicroscopy revealed that the strong alkaline environment required for the formation of sodium titanate nanoribbons did not affect the manganese oxidation state. In the next two steps, the ion-exchange process in the  $HCl(aq)$  solution followed by a thermal treatment in air lead to the formation of  $Mn^{2+}$  doped  $TiO_2$  nanoribbons. An analysis of the manganese content by X-ray photoelectron spectroscopy of several  $TiO_2$  nanoribbon samples calcinated in the temperature range from 400 to 700 °C, and the analysis performed at the  $Ti L_{2,3}$  and  $Mn L_{2,3}$  edges with electron-energy-loss spectroscopy showed that calcination at elevated temperatures induced the diffusion of manganese ions towards the nanoribbons' surface. However, the transformation of anatase nanoribbons to rutile nanoparticles was also accompanied by the partial oxidation of  $Mn^{2+}$  to  $Mn^{3+}$  and  $Mn^{4+}$ . Published in Umek et al., J. Phys. Chem C, Nanomaterials and interfaces, 2014.

### Critical properties of nanostructured and electrocaloric materials

Using direct measurements and a simple Kittel model it was shown that the negative electrocaloric effect should be observed in anti-ferroelectric materials. We also calculated the E-T phase diagram for anti-ferroelectrics and corresponding electrocaloric response as a function of temperature and field. By calorimetric and optical experiments we showed that the  $TGB_A$  phase (see Figure 9), which is analogous to the Abrikosov lattice vortex state in superconductors, can be stabilized by functionalized nanoparticles added to a highly chiral liquid crystal. The above results have been published in 6 articles in international scientific journals and a chapter published in a book published by Springer. Recently, published works on electrocalorics and the stabilization of TGB and blue phases have been cited more than 100 times in 2014 alone.

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

The investigations of the research program "Physics of Soft Matter, Surfaces, and Nanostructures" are focused on novel complex soft-matter systems and surfaces with specific functional properties. We investigated, in particular, liquid-crystalline elastomers and dendrimers as novel multifunctional materials, nematic colloids, molecular motors, soft-matter photonic crystals and novel synthetic or self-assembled micro- and nano-structures. The aim of the program is to understand the structural and dynamical properties of these systems, their interactions, their function at the molecular level, and self-assembly mechanisms in soft matter. The underlying idea is that it is possible to understand complex mechanisms, such as self-assembly, on a macroscopic level, using a simplified physical picture and models. In order to provide a comprehensive approach to the problem, the program combines both experimental and theoretical investigations, supported by modelling and simulations. Special emphasis is given to the possible electro-optic and medical applications.

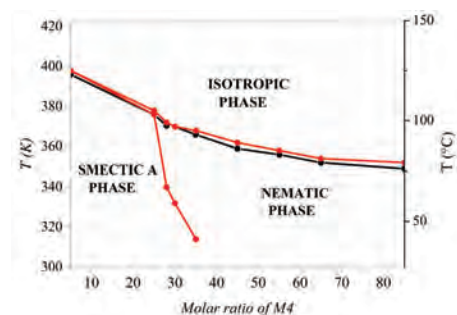


Figure 7: Phase diagram of a composite liquid single-crystal elastomer.

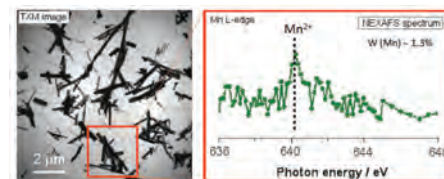


Figure 8: TEM image (left) and Mn L-edge NEXAFS spectrum (right) of  $Mn^{2+}$  doped  $TiO_2$  nanoribbons. Spectrum was acquired in the area marked with red square in the TEM image.

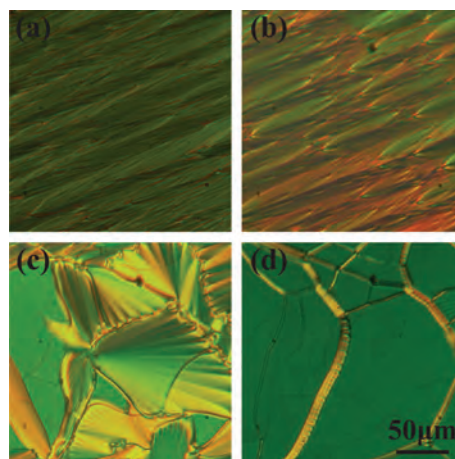


Figure 9: Texture of  $TGBA$  phase stabilized by nanoparticles (b). Other phases: smectic A (a), liquid vortex state (c) and the nematic phase (d).

**We have investigated the topology and photonics of liquid-crystal colloids and dispersions, and studied the motion of molecular motors. Tribological properties of nanomaterials and their safety were investigated; the structure of matter has been studied on the atomic level and the infrastructure for cold-atom physics was set up.**



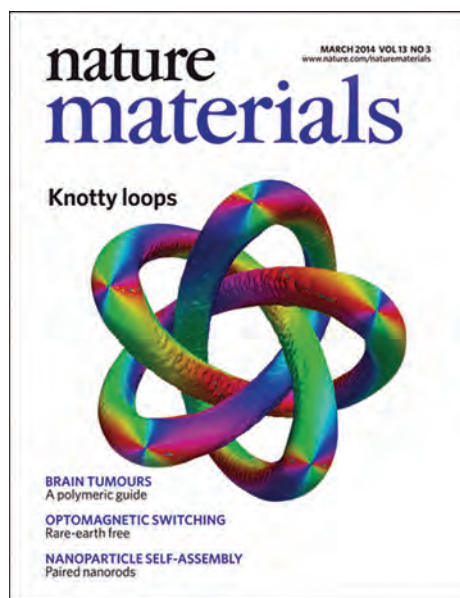


Figure 10: Front cover of a journal *Nature Materials*, showing a colloidal knot with a surface nematic director field in the case of degenerate planar anchoring. The cover picture was taken from A. Martinez, et al. *Nature Mater.* 13, 258-263 (2014).

### Mutually tangled colloidal knots and induced nematic defect loops

Micron-size particles in nematic liquid crystals induce complex distortions including topological defects, leading to effective inter-particle forces and consequently to self-assembled structures. In collaboration with Smalyukhs's group at UCO Boulder we theoretically and experimentally demonstrated the effect of 'colloidal knots' on the nematic field (Martinez et al., *Nature Materials* 2014). The micron-scale knotted particles created using two-photon photo-polymerisation induce nematic distortions that were analyzed by three-photon excitation fluorescence polarizing microscopy. Experimental results and computer simulations uncover numerous structures, for example, a knotted particle that induces perpendicular alignment of the director at its surface can lead to a pair of topological defect lines with the same knotted configuration as the particle. We suggest that the interplay between the topologies of the knotted particles and the knotted nematic field may provide the clue to a new types of self-assembled materials.

### Quasicrystalline tilings with nematic colloidal platelets

The inclusion of micron-sized faceted particles in liquid crystals opened up a rich new area of research. In collaboration with our former postdoc J. Dontabhaktuni we showed that in such a system the forces mediated by topological defects can form quasicrystalline structures (Dontabhaktuni et al. *PNAS* 2014). In a thin layer of an aligned nematic with the help of the Landau-de Gennes approach we found that surface defects in the nematic field can cause pentagonal platelets to join with their edges – which is different from stacking in an isotropic liquid, where edges can easily slide. This enables the formation of the Penrose tiling patterns. Interestingly, hierarchical structures can also be made where a given pentagonal platelet is substituted for a number of smaller ones of the same shape. We believe that this may be of interest for photonic metamaterials.

### Free-standing knots in confined chiral nematic fluids

Knotted fields are an emerging research topic relevant to different areas of physics where topology plays a crucial role. The recent realization of knotted nematic disclinations stabilized by colloidal particles raised the challenge of free-standing knots. We demonstrated the creation of free-standing knotted and linked disclination loops in the cholesteric ordering fields, which are confined as spherical droplets with normal surface anchoring (Seč et al., *Nature Comms.* 2014). Our approach, using free-energy minimization and topological theory, leads to the stabilization of knots via the interplay of the geometric frustration and intrinsic chirality (Beller et al. *Phys. Rev. X* 2014). Selected configurations of the lowest complexity are characterized by knot or link types, disclination lengths, and self-linking numbers (Čopar, *Phys. Rep.* 2014). The droplets with knots could be controlled by optical beams and may be of use for photonic elements.

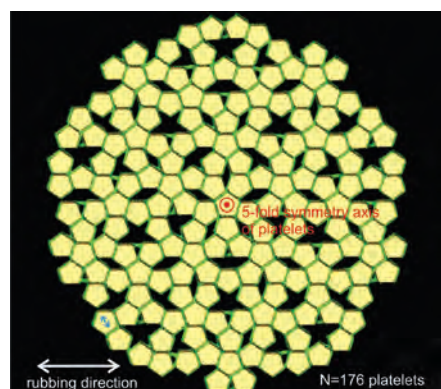


Figure 11: Colloidal quasicrystalline Penrose tiling assembled from 176 pentagonal particles in a nematic liquid crystal layer (J. Dontabhaktuni et al. *PNAS* 111, 2464 (2014)).

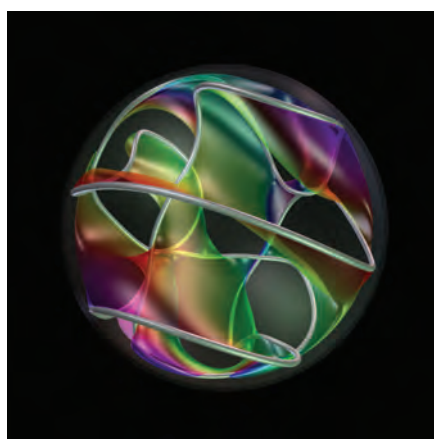


Figure 12: Homeotropic chiral nematic liquid-crystalline droplet with a single disclination loop exhibiting a trefoil knot. The Pontryagin-Thom surface where the directors are in the  $x$ - $y$  plane is colored according to the local orientation of the director field (D. Seč, S. Čopar and S. Žumer, *Topological zoo of free-standing knots in confined chiral nematic fluids*, *Nature Comms.* 5, 3057 (2014)).

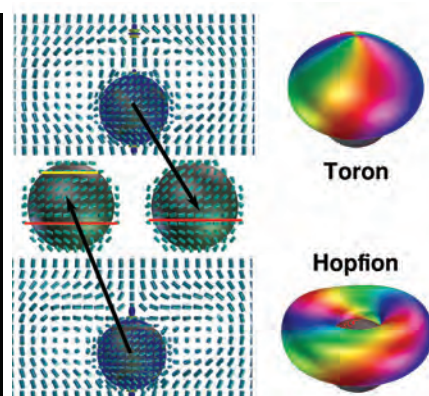


Figure 13: Soliton dressed colloidal particles in an untwisted thin cholesteric liquid crystalline layer. Toron and hopfion director fields appearing in the case of degenerate planar anchoring are visualized using cylindrical glyphs and Pontryagin-Thom surfaces (T. Porenta, S. Čopar, P. J. Ackerman, M. B. Pandey, M. C. M. Varney, I. I. Smalyukh and S. Žumer, *Topological switching and orbiting dynamics of colloidal spheres dressed with chiral nematic solitons*, *Scientific Rep.* 4, 7337 (2014)).

### Colloidal spheres dressed with chiral nematic solitons

Metastable liquid-crystalline configurations formed by defects, inclusions, and elastic deformations in forms of topological solitons are promising choices for building photonic crystals and metamaterials for new optical applications. Local optical modification of the director or colloidal inclusions into a moderately chiral nematic liquid crystal confined to a homeotropic cell creates localized multi-stable chiral solitons. In collaboration with Smalyukhs's experimental group at UCO in Boulder we induced solitons that "dress" the dispersed spherical particles treated for tangential degenerate boundary conditions, and performed controlled switching of their state using focused optical beams (Porenta et al., Scientific Rep. 2014). Two optically switchable distinct metastable states, toron and hopfion, bound to colloidal spherical micro-particles into nematic superstructures with different topological charges were investigated. Their structures examined using Q-tensor based numerical simulations and topological theory were compared to the profiles reconstructed from the experiments.

### Nematic colloids and photonics

We continued our investigations of nematic colloids for photonic applications by studying the polymerization of colloidal crystals, assembled by laser tweezers in the nematic liquid crystal. After polymerization, the colloidal crystals preserve the structure very well (Figure 14), and they are stable at elevated temperatures as well. After the removal of the polymer, SEM investigations (Figure 14b-e) reveal remnants of a polymer network, attached to the silica colloidal particles. Photo-polymerizable liquid crystals show an excellent potential for assembling the robust photonic superstructures for applications in photonics. Published in Mirri et al., Stabilisation of 2D colloidal assemblies by polymerisation of liquid crystalline matrices for photonic applications, *Soft Matter* 10, 5797 (2014). Ideas and concept of a new field of soft-matter photonics were presented in an invited article in *Liquid Crystals*, by I. Muševič (Integrated and topological liquid crystal photonics, *Liquid Crystals* 41, 418 (2014)).

### Interaction between nanoparticles and topological defects

We studied the nanoparticle-driven stabilization of Twist Grain Boundary A phase. By means of high-resolution ac calorimetry and polarizing optical microscopy we have demonstrated that surface-functionalized spherical CdSSe nanoparticles induce a twist-grain boundary phase when dispersed in a chiral liquid crystal (Figure 15). These nanoparticles can effectively stabilize the one-dimensional lattice of the screw dislocations, thus establishing the twist-grain boundary order between the cholesteric and the smectic-A phases. Moreover, a theoretical model that accounts for the trapping of nanoparticles in the defect cores was presented. In particular, we have shown that in addition to the Defect Core Replacement mechanism, also the saddle splay elasticity plays an important role (M. Trček et al., *Phys. Rev. E* 90, 032501 (2014)).

### Combined nanoparticle and UV-irradiation-driven nematic structural transitions

We studied experimentally and theoretically UV-irradiation and phospholipid stimulated bipolar-radial structural transitions of azoxybenzene nematic liquid crystals (NLCs) droplets dispersed in water (Figure 16). It was found that the UV-irradiation that triggered the trans-cis isomerisation of the LC molecules induced a structural transition to a radial configuration at the critical time  $t_c$ . In particular, we demonstrated that the critical UV-irradiation time  $t_c$  needed for the transition could, under appropriate conditions, sensitively depend on the concentration of phospholipid molecules. This demonstrated a proof-of-principle mechanism could be exploited for the development of sensitive detectors for specific nanoparticles (NPs), where value of  $t_c$  fingerprints concentration of NPs (V. Dubtsov et al., *Appl. Phys. Lett.* 105, 151606 (2014)).

### Molecular motors

We set a mechano-chemical model for the stepping dynamics of cytoplasmic dynein. The results of our elasto-mechanical description of a simplified model object, which mimics the basic properties of this complex molecule, show that such a dimeric molecule can synchronize the ATP hydrolysis cycles of its two heads to produce efficient processive coordinated stepping. The degree of synchronization of the two cycles is tuned by the strength of the coupling between the two heads of the dimer. With weaker coupling the heads lose synchrony and move in an uncoordinated manner with a much broader distribution of steps (Figure 17). In this case the high

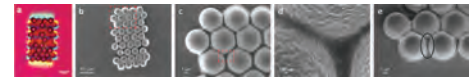


Figure 14: (a) Reflection-mode Optical microscopy images of a colloidal crystal of 5  $\mu\text{m}$  silica particles embedded in a polymerized nematic matrix after the non-polymerized LC was washed out, imaged between crossed polarizers with a retardation plate added; (b-d) SEM images of the same assembly at different magnifications; (e) SEM image of the assembly tilted by 12°. The blue ellipse indicates the region where the topological defect is expected to be observed.

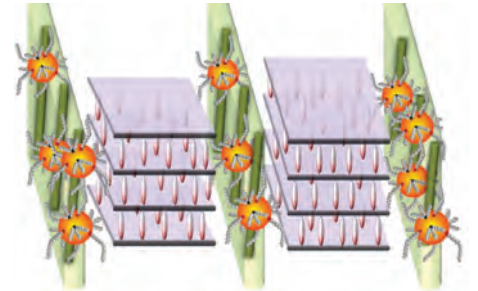


Figure 15: A simple schematic illustration of nanoparticles trapped to screw dislocations.

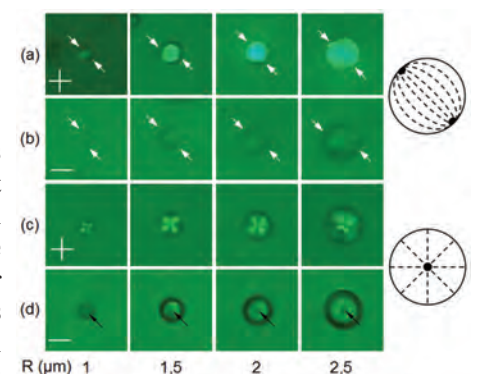


Figure 16: Microscopic images of liquid-crystal droplets in the absence of phospholipids and irradiation (a, b), in the presence of phospholipids (c, d), after 1 minute of irradiation in the absence of phospholipids (e, f).

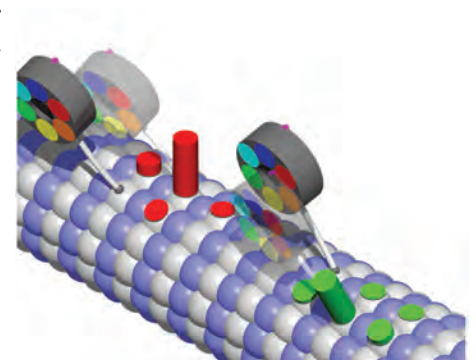


Figure 17: A model molecule of cytoplasmic dynein taking a step with its left or right head.



processivity is retained at the cost of a reduced velocity. These two scenarios seem to be realized in nature: the coordinated stepping for mammalian dyneins and the uncoordinated for dyneins of lower eucaryotes. We showed that the maximum force the loaded motor can withstand is largely limited by motor's processivity (A. Šarlah and A. Vilfan, *Biophysical Journal* 2014).

Non-processive molecular motors, such as muscle myosin, can only generate movement when coupled together in larger ensembles. Their ensemble velocity as a function of load has been the subject of many previous studies, but little was known about its dependence on the fuel ATP concentration. We showed that a model with several mechanical states can exhibit non-trivial dependencies that can reveal the sequence of conformational changes in a motor's cycle. The model also predicts the possibility of velocity reversal depending on the ATP concentration (A. Vilfan, *Interface focus* 2014). In addition, we contributed to the discussion about the origin of directional motion in myosin-V motors (A. Vilfan, *PNAS* 2014).

### Low-friction nanomaterials

In the paper "The formation of tribofilms of MoS<sub>2</sub> nanotubes on steel and DLC-coated surfaces" (M. Kalin et al. *Tribology Letters*, 55, 381-391 (2014)) we reported that the addition of the MoS<sub>2</sub> nanotubes to the oil can significantly reduce the coefficient of friction for the steel (up to 65 %) and the DLC-coated (up to 40 %) surfaces, in particular for the boundary-lubrication regime. The major difference between the steel and the DLC contacts is the extent to which the MoS<sub>2</sub>-based tribofilm covers the surface, which is 20 % in the case of the DLC/DLC contacts, but almost 40 % in the case of the steel/steel contacts. We found that the chemical and functional properties of the MoS<sub>2</sub>-based tribofilm are very similar, or even the same, for both the steel and DLC-coated surfaces.

### Nanosafety

In the paper "Sparklers as a nanohazard: size distribution measurements of the nanoparticles released from sparklers" (M. Remškar et al., *Air Quality, Atmosphere & Health* (2014)), we reported on the high concentrations of nanoparticles released during the indoor combustion of sparklers. Large proportions of the metals making up the sparking material are released into the atmosphere. The sparklers, which consisted of Ba(NO<sub>3</sub>)<sub>2</sub>, elemental Fe, and elemental Al, burned to produce BaAl<sub>2</sub>O<sub>4</sub>, BaAl<sub>2</sub>O<sub>6</sub>, and BaFe<sub>2</sub>O<sub>4</sub> and emitted nanoparticles that contained Ba, Fe, Al, Na, K, C, and O. The combustion of a single sparkler increased the concentration of nanoparticles in a cubic centimetre of air by at least 150 times, to 350,000/cm<sup>3</sup>. More than 10 % of the metals from the sparklers were released into the local atmosphere. The majority of these released particles were around 100 nm in size, but a substantial amount of them were found to be smaller than 20 nm in diameter (Figure 18). The closest position of the inlet to the sparkler (simulating a child's position) is the most hazardous because of the lowest degree of agglomeration of the nanoparticles. The nanoparticles remained in the atmosphere for several hours. Due to the small size and the chemical composition of the released NPs, and according to the published data on health hazards resulting from their inhalation, the use of sparklers as a children's entertainment should be reconsidered.

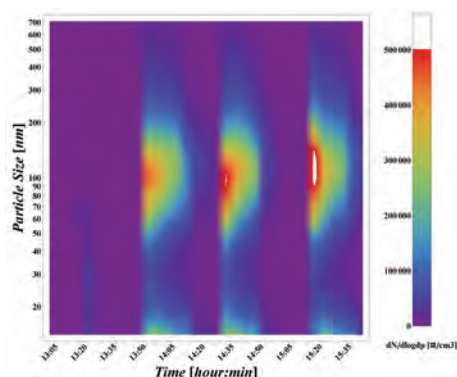


Figure 18: Nanoparticle pollution generated by a sparkler (a toy firework that emits little sparks).

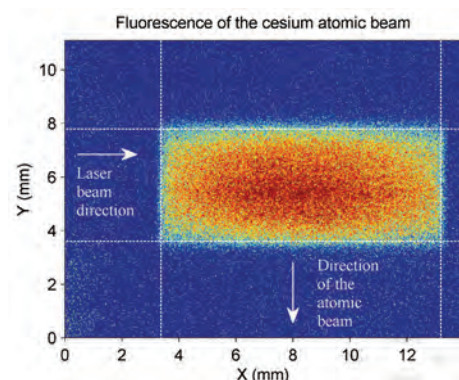


Figure 19: Fluorescence from a beam of Cs atoms in the main chamber of UHV apparatus for cold atoms

In collaboration with Chemical Office of Republic Slovenia we have built the website Nanoportal (<http://www.uk.gov.si/>, M. Remškar, U. Lavrenčič Štangar, D. Drobne, M. Pavlin) that represents the contact point for public interesting in nanotechnology and nanosafety. Besides basic information on specific properties of nanomaterials and monitoring tools, a list of researchers specialized on a particular nanomaterial is presented with the aim to strengthen the transfer of knowledge. We performed the monitoring of the pollution of air with nanoparticles in several industrial companies and at public sites using a professional particle sizer that enables a size distribution measurement.

### Ultra-cold atoms

The first experiments on detecting and characterizing a beam of Cs atoms in ultra-high vacuum apparatus for cold atoms were performed. Using a high-power diode laser locked to selected Cs atomic transition using a modulation transfer spectroscopy we observed fluorescence from the atomic beam in the main experimental chamber (Figure 19). Magnetic fields are being set up, which are needed to slow down and capture a large number of these atoms.

## III. Research programme Experimental biophysics of complex systems

In the program "Experimental biophysics of complex systems", the processes and structures of various complex biological systems are investigated, ranging from model systems to the structures in living cells, tissues

and small animals. Investigations also comprise the studies of the impact of numerous bioactive substances such as are toxins and drugs as well as a variety of materials from materials to medical materials on such biological systems. The research is recently focused on the better understanding of the structure of membrane compartments, domains, proteins, glyco-saccharides clusters, molecular structures of polymer gels, etc. and their interaction, accompanying the interaction of cell structures with new materials that enter into their natural environment. New spectroscopic and micro-spectroscopic techniques contribute to the better understanding of the organization of these supramolecular systems, complex cellular and tissue responses and open up new possibilities for the design of medical materials, especially for tissue regeneration, which is one of the main health issues among the aging population of the developed world. In addition, the research field is also directed to the optimization methods for the treatment of tumours, magnetic resonance imaging and the mathematical modelling of thrombolysis, the use of high-resolution magnetic resonance imaging to study materials. This method allows us to study different problems in forestry, wood industry, and food safety. We expect a lot from the development of new methods for measuring diffusion in porous materials, with which we will be able to tell a lot about the microscopic structure of porous materials.

The **cell-material interaction studies**, especially from the viewpoint of bioactivity and biocompatibility, are undoubtedly one of the hottest biophysics research topics. By new micro-spectroscopies we efficiently address the problem of nanoparticles and nanofibres uptake into the cell or the model membrane. Uptake into and through the membrane was proven by the FMS-FRET-experiments acquired on model membranes. We also explored the effect of the properties of nanoparticles such as their size and their surface properties on the interaction of the nanoparticles with biological systems. As a result, some methods to control the size of and surface properties of the nanoparticles have also been undertaken.

Through the studies of the **conformational entropy** of the spin labels incorporated into lipid membranes, significant progress in the development of experimental methods for studying the interaction of nanoparticles with biological systems was shown. Conformational entropy is otherwise a method that has long been used for the theoretical identification of the dynamics of proteins, DNA and other polymers, but its accurate experimental determination has been hampered due to the correlated molecular dynamics. We have shown that the correlated molecular dynamics can be estimated directly from the temperature dependence of local conformational entropy, which can then be used to determine the correct conformational entropy of the entire molecule. The work was published in a journal with the impact factor of 6.7 (*J. Phys. Chem. Lett.*, 2014, 5 (20), pp 3593-3600). This method can be useful in a number of experimental techniques and thus provides an additional insight into the physical properties of various biomolecules.

**Fluorescence microspectroscopy** is the experimental method by which the fluorescent spectra of each microscopic sample volume element are acquired, revealing the physical properties of the surrounding environment on a molecular scale. Implementation of this method to the nanoparticle uptake problem allows us to analyse the rate and the mechanism of the titanate nanotubes transition into giant liposomes. Special approaches that employ the fluorescence resonance energy transfer concept and the fluorescent labelling of both the nanoparticles and the membranes revealed the accumulation of the nanoparticles onto the model biological membranes. The same method was also used in the study of **interaction between cells and macro-structured polymeric scaffolds** as potential tissue engineering materials, by which morphological properties of the latter and cell ingrowth with its morphology were measured through fluorescent detection. Cell ingrowth was compared and correlated with the molecular and macroscopic properties of the scaffolds, which was done by the analysis of molecular dynamics of polymers by **spin labeling EPR spectroscopy** and rheology. The study was published in a journal with an impact factor 5.9 (*ACS Appl. Mater. Interfaces*, 2014 6 (18), pp 15980-15990). Further interactions between cell and biomaterials have been studied through the analysis of the dynamics and strength of cell adhesion to these tissue-engineering scaffolds by using a system of **optical tweezers** (sent for publication). Fluorescence microspectroscopy was also applied to **present the effect of antimicrobial technology NANO4AB** developed in our laboratory (Figure 20) to identify bacteria and nanomaterials with an optical set-up that allows us to distinguish them despite the fact that these objects are close to or below the resolution of the microscopy.

Since the properties of **nanoparticles** play an important role in the interaction with biological systems, we started a collaboration with the laboratory of Nobel Prize winner Oliver Smithies from the University of North Carolina and developed two methods for the synthesis of gold nanoparticles with the controlled size from 3 nm to 30 nm and with an optionally functionalized surface. This work was published in the journal *Langmuir* with an

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**Our studies have shown that the molecular motional correlation can be estimated directly from the temperature dependence of the local conformational entropy, which can then be used to determine the correct conformational entropy of the entire molecule. We have developed a method of NMR imaging that allows imaging of an electric field during electroporation in vivo. Data about the electric field are crucial for monitoring treatment with electroporation.**

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impact factor of 4.4 (Langmuir 11;30(44):13394-404). Based on this work, we were invited to prepare a paper for the journal, Journal of Visualized Experiments (JoVE).

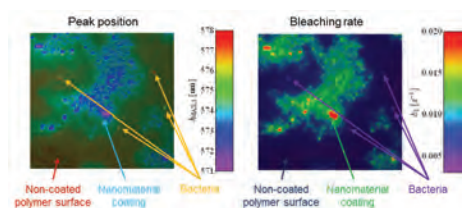


Figure 20: Fluorescent microspectroscopy was used to demonstrate the anti-microbial properties of our technology NANO4AB and the identification of bacteria and nanomaterials using an optical set-up. The image on the left is coding the peak of the emission spectra; the image on the right is coding the speed of the bleaching of fluorophore. One can clearly resolve the nanomaterial and bacteria.

Our results indicate that the formation of lipid corona is possible, where the nanoparticle is wrapped by a lipid membrane. We hypothesize that such lipid-wrapped nanoparticles may resemble lipid vesicles derived from platelets, usually known as “microparticles”. An important characteristic of microparticles is that a key reaction of **blood coagulation** takes place on them, the **activation of factor Xa**. Microparticles are membranous vesicles in blood derived from activated platelets or other cells containing the phospholipids of the parent membranes. Microparticles are detectable in normal human blood and are increased in patients with coagulation abnormalities. We therefore studied the activity of an enzyme factor Xa and found that the regulation of the activity of Factor Xa depends critically on the concentration of calcium in the plasma and that this process is likely to be physiologically important in the initial stage of blood clotting. This work was published in the Biochemical Journal with impact factor of 4.7 (Biochem. J. (2014) 462, 591-601) in collaboration with another group of researchers from the University of North Carolina. We also showed that a similar process occurs on activated platelets, which further confirms the physiological role of factor Xa activity on lipid membranes (accepted for publication in the Biochemical Journal).

We also focused on the problem of **diffusion in one- and two-dimensional cases** efficiently tackled by Adaptive Bias Force Molecular dynamics and created a generally applicable software package for determining multidimensional position-dependent diffusion coefficients (J. Chem Phys 140, no. 8, 084109; github.com/lbf-ijis/DiffusiveDynamics). With the obtained diffusion surface and a known free-energy surface, diffusive trajectories can be generated. Using this approach the time scale of molecular dynamics, typically a few 100 nanoseconds, can be extended to several 100 microseconds (for the 1D or 2D subspace of interest). By this approach, we studied the side-chain motion of spin labelled  $\alpha$ -helices in the membrane and improved the description of the lipid effect within the side-chain conformational space modelling of proteins (CSM) which drastically reduces the computational time needed for determining the size of the side-chain conformational space. This allowed us to apply the improved CSM method on the **structure characterization of the anti-microbial peptide  $\beta$ -defensin** in water and in SDS-micelles. By comparing experimental side-chain conformational spaces, obtained from EPR spectra and calculated side-chain conformational spaces using the improved CSM method, we were able to determine the insertion of the peptide into the membrane and estimate the local diffusion of the spin-labelled side chain at each mutant position.

In the field of the design and the **synthesis of labels** (nitroxide, fluorophore and combined nitroxide-fluorophore), the research was focused on the environmentally sensitive fluorophores, especially on the surrounding polarity and hydration. We were able to synthesize a small series of fluorophores based on 7-(diethylamino)coumarin, where the bathochrome shift in both the excitation and emission spectrum was achieved due to rational planning of the synthesized fluorophores. Fluorescent spectra measured in different solvents showed very large to moderate sensitivity of different fluorophores to the surrounding polarity, while all showed high photostability. These findings were published in Tetrahedron Letters journal (Tetrahedron Letters (2014), 55 (44), 6044-47). To investigate the differences in polarity within the membrane associated with different membrane processes, new membrane probes are designed based on the synthesized environmentally sensitive fluorophores. We furthermore continued the synthesis and evaluation of rhodamine-type pH-sensitive fluorescent labels for the identification of pH-change in the environment, more specifically for the study of cell organelles with lower pH values.

We developed a **MR imaging method** enabling the imaging of an electric field during electroporation *in vivo*. The information on the electric field is essential for **monitoring of electroporation treatment** (Figure 21). Plasmin is a direct-acting thrombolytic agent with a favourable safety profile upon intra-arterial delivery in pre-clinical and phase I studies. However, the **thrombolytic efficacy of plasmin**, relative to that of rt-PA, remains to be established. We conducted a study in which the differences in thrombolysis between clots exposed to equimolar concentrations of plasmin and rt-PA after partial vessel recanalization were tested in a model system. Model blood clots were prepared in glass chambers enabling direct observation by dynamic optical microscopy. The incubation of clots with plasmin or rt-PA, allowing for the initial biochemical clot degradation, was followed by “flushing” the clots with a tangentially directed plasma flow devoid of a thrombolytic agent, mimicking blood flow after partial vessel recanalization. The acquired images were analysed for non-dissolved blood clot area as a function of time. With both thrombolytic agents, the relative clot area decreased rapidly in the first 30 s after the initiation of perfusion due to “flushing” the degraded clot fragments. In the following minutes the clot size showed a linear time dependence: after incubation with plasmin the clot size did not change substantially any more, while after incubation with rt-PA the clot size continually decreased. The slopes of the regression lines differed significantly. The thrombolytic action of the plasmin was terminated rapidly by contact with flowing blood plasma, while the thrombolytic action of rt-PA was prolonged. The findings of this study were published in the journal Thrombosis Research.



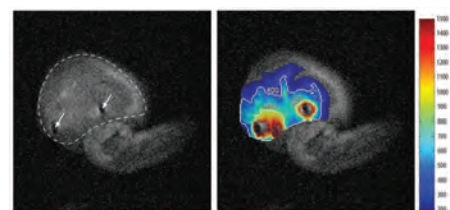
Magnetic resonance imaging allows monitoring of the distribution of electric current density in the conductive samples. By using current images in several different arrangements of electrodes, it is possible to determine the **electrical conductivity of the sample** and consequently also the electric field for a given electrode arrangement. This is of paramount importance **in electroporation**, which is a method in which by the use of high voltage the cell membrane is a tissue that is made temporary permeable and therefore absorbs more drugs than normally, as for example anti-cancer drugs. In this area, we worked with a group of prof. Damian Miklavčič from the Faculty of Electrical Engineering. Within this collaboration, we conducted a number of important *in vivo* MRI experiments of current distribution during electroporation and were able to determine the presence and extent of the region of reversible electroporation *in vivo*. In the electroporated region, the tissue cells open for a short time and the anticancer drug can enter the cells and stays there since the cells close again. Cancer cells in this process die, while most of healthy cells should survive. In our experiments, instead of the anticancer drug a MRI contrast agent was injected into experimental animals. In the region of reversible electroporation the contrast agent remained in the tissue also after several days, while it was not present at that time in other tissues that were not reversibly electroporated. Thus, we were able to detect the region of reversible electroporation and also to compare its extent with predictions for the region that were done based on calculations of the electric field strength on the basis of the measured current density distribution. We published the findings of this study in the distinguished journal *Radiology*.

Our collaboration with the group of Prof. Eung Je Woo from Kyung Hee University in Korea led to some interesting results in the field of advanced methods for **MR imaging of electrical conductivity**. Among other results we also developed a new imaging method that allows simultaneous tissue conductivity mapping at the radiofrequency (RF) range and at near zero frequency (DC) range. The method was tested on test samples as well as on experimental dogs. The result of the study are published in *IEEE transactions on medical imaging*.

In the journal *Angewandte Chemie International Edition* an article entitled "Selective Targeting of Tumor and Stromal Cells By a Nanocarrier System Displaying Lipidated cathepsin B inhibitor" was published in collaboration with department B1. A novel system for targeted drug delivery to tumours (LNC-NS-629) was developed. The system consists of nanoliposomes with incorporated lipidated CtsB specific inhibitor allowing targeting of cathepsin B (CtsB), a cysteine proteinase that is specifically up-regulated in cancers and translocated from its intracellular lysosomal locations to the cell surface and/or secreted into the extracellular milieu by tumour and tumour-associated stromal cells. The basis of the system are nanoliposomes, inside which there is enough space for small and large molecules, i.e., for the encapsulation of a drug or a diagnostic agent, such as a contrast agent for magnetic resonance imaging (MRI). In the paper T1-weighted MRI imaging *in vivo* was used to demonstrate the efficiency of the LNC-NS-629 system containing Magnetvist (T1 MRI contrast agent) targeting to the tumour microenvironment. The MRI images showed significant enhancement of contrast at the tumour site only 1 hour post-administration of the system. After 24 hours, the increased signal in the area of the tumour was still observed, reflecting the slower elimination of the LNC-NS-629 system with Magnetvist than in the case of Magnetvist alone. The system has been tested on healthy animals, where no accumulation of LNC-NS-629 was observed on the MRI images, indicating the rapid elimination of the LNC-NS-629 system from a healthy organism. It was shown that the new system has the potential to increase the efficacy of cancer diagnosis and treatment.

Our research has been supported by a number of international projects financed by the European Union within the 6th and 7th Frameworks. It was also supported within the bilateral Slovenian-USA, Slovenian-German and Slovenian-Greek and other scientific cooperations. In 2014, the department had cooperations with 108 partners from Slovenia and abroad. Among them:

- The high magnetic field centres in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field 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 Saarbrücken 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 Delbrück Center for Molecular medicine in Berlin
- The Dartmouth Medical School, Hanover, NH, USA



*Figure 21: MR EIT images demonstrate electric field distribution in a mouse tumour during electroporation. (a) The tumour t1 (marked with a dashed white line) is situated on an animal leg in this T1-weighted image, acquired in the section perpendicular to the electrodes. Locations of the two inserted electrodes are marked with arrows. (b) The electric field distribution in the tumour, obtained with MR EIT, was superimposed onto the T1-weighted image acquired before the application of electric pulses. A white contour line encloses an area exposed to an electric field strength between reversible (400 V/cm) and irreversible (900 V/cm) electroporation threshold values. Tumour cells located outside the area are either irreversibly electroporated (the area close to the electrodes) or remain unelectroporated (the area toward the tumour boundary).*

- The Mayo Clinic, Rochester, USA
- Kyung Hee University, Suwon, Korea
- Technische Universität Ilmenau, Ilmenau, Germany
- Elettra Sincrotrone Trieste, Trieste, Italy
- University of North Carolina at Chapel Hill
- Max-Delbrück-Centrum für Molekulare Medizin (MDC)

made the above studies possible.

### Some outstanding publications in 2014

1. Zorko, A., Adamopoulos, O., Komelj, M., Arčon, D., Lappas, A.: Frustration-induced nanometre-scale inhomogeneity in a triangular antiferromagnet. *Nature Comms* 5, 3222 (2014).
2. Koželj, P., Vrtnik, S., Jelen, A., Jazbec, S., Jagličič, Z., Maiti, S., Feuerbacher, M., Steurer, W., Dolinšek, J.: *Phys. Rev. Lett.* 113, 107001 (2014).
3. Pirc, R., Rožič, B., Koruza, J., Malič, B., Kutnjak, Z.: Negative electrocaloric effect in antiferroelectric  $\text{PbZrO}_3$ . *Europhysics Letters* 107, 17002-1-5(2014).
4. Martinez, A., Ravnik, M., Lucero, B., Visvanathan, R., Žumer, S., Smalyukh, I. I.: Mutually tangled colloidal knots and induced defect loops in nematic fields, *Nature Mater.* 13, 258-263 (2014).
5. Seč, D., Čopar, S., Žumer, S.: Topological zoo of free-standing knots in confined chiral nematic fluids, *Nature Comms.* 5, 3057 (2014).
6. Dontabhaktuni, J., Ravnik, M., Žumer, S.: Quasicrystalline tilings with nematic colloidal platelets, *Proceedings of the National Academy of Sciences of the United States of America* 111, 2464 (2014).
7. Čopar, S.: Topology and geometry of nematic braids, *Phys. Rep.* 538, 1-37 (2014).
8. Vilfan, A.: Myosin directionality results from coupling between ATP hydrolysis, lever motion, and actin binding. *Proceedings of the National Academy of Sciences of the United States of America* 111, E2076 (2014).
9. Urbančič, I., Ljubetič, A., Štrancar, J.: Resolving Internal Motional Correlations to Complete the Conformational Entropy Meter. *J. Phys. Chem. Lett.* 5, 3593-3600 (2014).
10. Podlipec, R. et al.: Molecular Mobility of Scaffolds' Biopolymers Influences Cell Growth. *ACS Appl. Mater. Interfaces* 6, 15980-15990 (2014).
11. Mikhaylov, G. et al.: Selective targeting of tumor and stromal cells by a nanocarrier system displaying lipidated cathepsin B inhibitor. *Angew. Chem. Int. Ed Engl.* 53, 10077-10081 (2014).

### Some outstanding publications in 2013

1. Vallejos, S., Umek, P., Stoycheva, T., Annanouch, F., Llobert, E., Correig, X., de Marco, P., Bittencourt, C., Blackman, C.: Single-step deposition of Au- and Pt-nanoparticle-functionalized tungsten oxide nanoneedles synthesized via aerosol-assisted CVD, and used for fabrication of selective gas microsensor arrays. *Advanced Functional Materials* 23, 1313-1322(2013).
2. Gradišek, A., Bomholdtravnsbaek, D., Vrtnik, S., Kocjan, A., Lužnik, J., Apih, T., Jensen, T., Skripov, A. V., Dolinšek, J.: NMR study of molecular dynamics in complex metal borohydride  $\text{LiZn}_2\text{BH}_{45}$ . *Journal Phys. Chem. C* 117, 21139-21147(2013).
3. Pregelj, M., Zorko, A., Zaharko, O., Jeglič, P., Kutnjak, Z., Jagličič, Z., Jazbec, S., Luetkens, H., Hillier, A. D., Berger, H., Arčon, D.: Multiferroicity in the geometrically frustrated  $\text{FeTe}_2\text{O}_5\text{Cl}$ . *Phys. Rev. B* 88, 224421-1- 10(2013).
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5. Jampani, V. S. R., Škarabot, M., Čopar, S., Žumer, S., Muševič, I.: Chirality screening and metastable states in chiral nematic colloids. *Phys. Rev. Lett.* 110, 177801-1-5(2013).
6. Novak, S., Drobne, D., Vaccari, L., Kiskinova, M. P., Ferraris, P., Birarda, G., Remškar, M., Hočevar, M.: Effect of ingested tungsten oxide ( $\text{WO}_x$ ) nanofibers on digestive gland tissue of Porcellio scaber (Isopoda, Crustacea) : fourier transform infrared (FTIR) imaging. *Env. Sci. & Tech.* 47, 11284-11292(2013).
7. Bajd, F., Serša, I.: Mathematical modeling of blood clot fragmentation during flow-mediated thrombolysis. *Bioph. Journal* 104, 1181-1190(2013).
8. Urbančič, I., Ljubetič, A., Arsov, Z., Štrancar, J.: Coexistence of probe conformations in lipid phases : a polarized fluorescence microspectroscopy study. *Bioph. Journal* 105 919-927(2013).

## Awards and appointments

1. Simon Čopar: Jožef Stefan Golden Emblem Prize
2. Simon Čopar: Glenn Brown Prize, International Liquid Crystal Society
3. Slobodan Žumer: Honoured member of the International Liquid Crystal Society, International Liquid Crystal Society

## Organization of conferences, congresses and meetings

1. Alpine NMW Workshop, Bled Slovenia, 18-21 September 2014
2. Midterm Review Meeting, JSI, Ljubljana, Slovenia, 10-11 April 2014

## INTERNATIONAL PROJECTS

1. MERCK - AFM Investigations  
Asst. Prof. Miha Škarabot  
Merck KGaA
2. Development of Curved LCD Shutter  
Prof. Igor Muševič  
Kimberly-Clark
3. 7FP - LEMSUPER; Light Element Molecular Superconductivity: An Interdisciplinary Approach  
Prof. Denis Arčon  
European Commission
4. 7FP - ESNSTM; Electron Spin Noise Scanning Tunneling Microscopy  
Prof. Janez Dolinšek  
European Commission
5. 7FP - NanoMag; Magnetic Nanoparticles and Thin Films for Spintronic Applications and High Performance Permanent Magnets  
Prof. Janez Dolinšek  
European Commission
6. 7FP - NEMCODE; Controlled Assembly and Stabilisation of Functionalised Colloids in Nematic Liquid Crystals  
Prof. Igor Muševič  
European Commission
7. 7FP - LIVINGLASER; A Laser Made Entirely of Living Cells and Materials Derived from Living Organisms  
Prof. Igor Muševič  
European Commission
8. 7FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability  
Prof. Maja Remškar  
European Commission
9. 7FP - SIMDALEE2; Sources, Interaction with Matter Detection and Analysis of Low Energy Electrons 2  
Prof. Maja Remškar  
European Commission
10. COST MP1003; ESNAM - European Scientific Network for Artificial Muscles  
Prof. Boštjan Zalar  
COST Office
11. COST MP1201; Rational Design of Hybrid Organic-Inorganic Interfaces: The Next Step Towards Advanced Functional Materials  
Dr. Polona Umek  
COST Office
12. Exotic Electronic Properties arising from Geometrical Symmetry  
Prof. Denis Arčon  
Slovenian Research Agency
13. Elastically Tuned Soft Nanocomposites  
Prof. Samo Kralj  
Slovenian Research Agency
14. Liquid Crystals Blue Phases in Confined Geometries: Structure, Optical Properties and Photonic Applications  
Prof. Igor Muševič  
Slovenian Research Agency
15. Novel Polymeric and Ionomeric Materials with Giant Dielectric and Electrocaloric Response  
Asst. Prof. Vid Bobnar  
Slovenian Research Agency
16. Physiological Role of Factor Xa and Protein S in Coagulation and Inflammation  
Dr. Tilen Koklič  
Slovenian Research Agency
17. Key Role of Magnetic Anisotropy in Low-dimensional Spin Systems  
Dr. Andrej Zorko  
Slovenian Research Agency
18. Hybrid Solar Cell Based on Conducting Polymers and 1D Nanostructured TiO<sub>2</sub>

- Dr. Polona Umek  
Slovenian Research Agency
19. Solar Cell Application of Rf Rotating Plasma Modified Inorganic Nanotubes  
Prof. Maja Remškar  
Slovenian Research Agency
  20. Low Dimensional Structures of Metal Sulfides and Selenides for Use in Transistor Electronics  
Prof. Maja Remškar  
Slovenian Research Agency
  21. Local Studies of Frustrated Quantum Antiferromagnets  
Dr. Andrej Zorko  
Slovenian Research Agency
  22. Crystal and Electronic Structure of Quasi One-dimensional Transition-metal Chalcogenides  
Dr. Erik Zupanič  
Slovenian Research Agency

## RESEARCH PROGRAMS

1. Experimental Biophysics of Complex Systems  
Prof. Igor Serša
2. Physics of Soft Matter, Surfaces, and Nanostructures  
Prof. Slobodan Žumer
3. Magnetic Resonance and Dielectric Spectroscopy of "Smart" New Materials  
Prof. Janez Dolinšek

## R & D GRANTS AND CONTRACTS

1. Optical Microresonators based on Liquid Crystals  
Prof. Igor Muševič
2. New Metallic Materials for Thermal Storage of Digital Information  
Prof. Janez Dolinšek
3. Design, Formulation and Characterization of Biomimetic Nanocomposite Systems for Effective Tissue Regeneration  
Dr. Mojca Urška Mikac
4. Theory of the Nematic Nanodroplet and Ordering of DNA, Encapsidated in Simple Viruses  
Asst. Prof. Andrej Vilfan
5. Collective and Molecular Dynamics of Photosensitive Liquid Crystal Elastomers  
Prof. Boštjan Zalar
6. Optimization Strategies in Biological and Artificial Microfluidic Systems  
Asst. Prof. Andrej Vilfan
7. Thermophoretic Guidance, Accumulation and Sorting of Biomolecules in Microfluidic Devices  
Prof. Igor Muševič
8. Thermophoretic Guidance, Accumulation and Sorting of Biomolecules in Microfluidic Devices  
Asst. Prof. Andrej Vilfan
9. Intra-pocket-targeted Nanomedicines for Treatment of Periodontal Disease  
Prof. Maja Remškar
10. Use of Green Energy Sources: New Functional Nanomaterials on the Base of Polyoxometalates and TiO<sub>2</sub> Nanostructures for Production of Hydrogen by Catalytic Oxidation of Water -NANOleaf  
Dr. Polona Umek
11. New Advanced Electrocaloric Materials for Novel Environmentally Friendly Dielectric Refrigeration Technology  
Prof. Zdravko Kutnjak
12. The Textural Analysis of Spatiotemporal Changes for Breast Lesions Diagnosis on Ultrafast Breast MRIs  
Prof. Igor Serša

13. Role of Calcium and Lipid Membranes in Survival of Critically Ill Patients  
Dr. Tilen Koklič
14. Oligomers of Amyloidogenic Proteins from A to Z: Biophysical Properties, Structure, Function and Mutual Interactions  
Asst. Prof. Miha Škarabot
15. Selective and Hipersensitive Microcapacitive Sensor System for Targetted Molecular Detection in the Atmosphere  
Prof. Igor Muševič
16. Behaviour of Disipative Systems under Extreme Termo-Mechanical Loading  
Dr. Andrej Zorko
17. New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics  
Prof. Boštjan Zalar
18. Micro-electromechanical and Electrocaloric Layer Elements  
Prof. Zdravko Kutnjak
19. Water Exclusion Efficacy, Measure for Prediction of Wood Performance against Wood Decay Fungi  
Prof. Igor Serša
20. A spectrometer for Automatic <sup>14</sup>N Nuclear Quadrupole Resonance Characterization of New Substances  
Dr. Alan Gregorovič
21. Light-controlled Layer-by-layer Formation of Scaffolds for Faster Tissue Regeneration  
Dr. Iztok Urbančič
22. New Polymer and Ceramic Materials for Potential Use in Capacitors  
Dr. Andreja Eršte
23. Implementation Services MRI Recording Samples  
Prof. Igor Serša
24. TABANA: Targeting AntimicroBial Activity via Micro/Nano-structured Sufaces for Civil Applications  
Prof. Janez Štrancar
25. NQR Measurements of Active Pharmaceutical Ingredients  
Dr. Alan Gregorovič
26. Nanomaterials and Scaffolds Preparation and Characterization  
Prof. Janez Štrancar
27. Analysis with NQR (Nuclear Quadrupolar Resonance) Method  
Prof. Igor Muševič
28. Irradiation and Analysis of Si Samples  
Prof. Igor Muševič
29. SCOPES; Spin-liquid and Spin-ice States in Frustrated Rare-earth and Transition Metal Spinels  
Dr. Matej Pregelj
30. Irradiation and Analysis of Nano Si Samples  
Asst. Prof. Vid Bobnar

## NEW CONTRACTS

1. CONPHIRMER: Counterfeit Pharmaceuticals Interception using Radiofrequency Methods in Realtime  
Asst. Prof. Tomaž Apih  
Jožef Stefan International Postgraduate School
2. Cooperation within the R&D Program of the Company Akripol  
Prof. Maja Remškar  
Akripol, d. o. o.
3. Research and Development Agreement  
Prof. Igor Muševič  
Balder, d. o. o.

## VISITORS FROM ABROAD

1. Dr. Jun-ichi Fukuda, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, 18 December 2013-11 February 2014, 12-25 October 2014
2. Dr. Vassilios Tzitzios, National Centre of Scientific Research "Demokritos", Athens, Greece, 2-16 February 2014
3. Dr. Mutsuo Igarashi, Gunma National College of Technology, Department of Applied Physics, Maebashi, Japan, 20 February-4 March 2014, 28 April-5 May 2014, 20-26 August 2014
4. Dr. Anna Ryzhkova, ASML, Eindhoven, Netherlands, 26 February-6 March 2014, 3-6 July 2014; 2-6 November 2014
5. Dr. Marek Mihalkovič, Slovak Academy of Sciences, Institute of Physics, Bratislava, Slovakia, 4-6 March 2014
6. Prof. Katsumi Tanigaki, WPI-AIMR, Tohoku University, Materials Physics, Nano Solid-State Physics, Department of Physics, Sendai, Japan, 12-14 March 2014
7. Nerea Sebastián, Ugartheche, Dpto. Física Aplicada II, Facultad de Ciencia Y Tecnologia, Universidad del Pais Vasco UPV/EHU, Leioa, Spain, 24 March-30 April 2014
8. Dr. Rama Rao Pratihba, Raman Research Institute, Soft condensed Matter Lab, Bangalore, India, 31 March-30 April 2014
9. Marta Vidrih, University of Copenhagen, School of Business, Copenhagen, Denmark, 2-16 April 2014
10. Dr. Adam Ostrowski, Institute of Molecular Physics, Poznan, Poland, 9-12 April 2014
11. Dr. David Wilkes, Merck, Darmstadt, Germany, 12-13 May 2014
12. Dr. Barbara Piuze, Alltek Alltek Innovation S.r.l., Corno di Rosazzo, Italy, 15 May-14 September 2014
13. Dr. Sefer Avdić, Faculty of Mathematics and Natural Sciences of the University of Pristina, Pristina, 20-25 May 2014
14. Dr. Surajit Dhara, University of Hyderabad, School of Physics, Andhra Pradesh, India, 1-27 June 2014
15. Nezahat Can, Mustafa Kemal University, Turkey, 26 June-30 September 2014
16. Dr. Ivana Capan, Institut rudjer Bošković, Zagreb, Croatia, 10-13 July 2014, 25-27 October 2014
17. Dr. Mirta Herak, Institute of Physics, Zagreb, Croatia, 15 July 2014, 13-18 October 2014, 24-28 November 2014
18. Dr. Venkata Subba Rao Jampani, Max Planck Institute, Goettingen, Germany, 24 July-12 August 2014
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24. Yang Xia, Oakland University, Department of Physics, Rochester-MI, USA, 18-21 September 2014
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27. Dr. Magdalena Wencka, Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland, 6 October-5 November 2014
28. Dr. Carla Bittencourt, University of Mons, Belgium, 18-22 October 2014
29. Dr. Emmanuelle Lacaze, Institute des nano-Sciences de Paris, France, 2-5 December 2014
30. Dr. Sergey Zybtev, V.A. Kotelnikov Institute of Radioengineering and Electronics of Russian Academy of Sciences, 13-19 December 2014

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29. Asst. Prof. Zoran Arsov
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62. Bojan Marin\*, M. Sc.
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79. Andreja Berglez, B. Sc., left 24. 11. 14
  80. Dražen Ivanov
  81. Janez Jelen, B. Sc.
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  88. Ana Sepe, B. Sc.
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# BIBLIOGRAPHY

## ORIGINAL ARTICLE

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2. Nina Bizjak, Franci Bajd, Jernej Vidmar, Aleš Blinc, Maja Pohar Perme, Victor J. Marder, Valery Novokhatny, Igor Serša, "Direct microscopic monitoring of initial and dynamic clot lysis using plasmin or rt-PA in an in vitro flow system", *Thromb. res.*, vol. 133, issue 5, pp. 908-913, 2014.
3. Ksenija Cankar, Lidija Nemeth, Franci Bajd, Jernej Vidmar, Igor Serša, "Discrimination between intact and decayed pulp regions in carious teeth by ADC mapping", *Caries Res.*, vol. 48, no. 5, pp. 467-474, 2014.
4. Goran Casar, Xinyu Li, Qiming M. Zhang, Vid Bobnar, "Influencing dielectric properties of relaxor polymer system by blending vinylidene fluoride-trifluoroethylene-based terpolymer with a ferroelectric copolymer", *J. appl. phys.*, vol. 115, no. 10, pp. 104101-1-10410-5, 2014.
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6. Simon Čopar, Miha Ravnik, Slobodan Žumer, "Janus nematic colloids with designable valence", *Materials (Basel)*, vol. 7, iss. 6, pp. 4272-4281, 2014.
7. Erik Čuk, Matjaž Gams, Matej Možek, Franc Strle, Vera Maraspin-Čarman, Jurij F. Tasič, "Supervised visual system for recognition of erythema migrans, an early skin manifestation of lyme borreliosis", *Stroj. vestn.*, vol. 60, no. 2, pp. 115-123, Feb. 2014.
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13. Andrej Fabjan, Fajko Bajrovič, Bojan Musizza, Jernej Vidmar, Martin Štručl, Marjan Zaletel, "Study of neurovascular coupling during cold pressor test in patients with migraine", *Cephalalgia*, vol. 34, iss., pp. 1-10, 2014.
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15. Jun-ichi Fukuda, Slobodan Žumer, "Exotic defect structures and their optical properties in a strongly confined chiral liquid crystal", In: 15th Topical Meeting on Optics of Liquid Crystals, OLC 2013, September 29-



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  21. Simon Jazbec, Stanislav Vrtnik, Zvonko Jagličič, Shiro Kashimoto, Jovica Ivkov, Petar Popčević, Ana Smontara, Hae Jin Kim, Jin Gyu Kim, Janez Dolinšek, "Electronic density of states and metastability of icosahedral Au-Al-Yb quasicrystal", *J. Alloys Compd.*, vol. 586, pp. 343-348, 2014.
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## SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK

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2. Aleš Mohorič, Vito Babič, *Fizika 1: učbenik za fiziko v 1. letniku gimnazij in štiriletnih strokovnih šol*, 1. izd., Ljubljana, Mladinska knjiga, 2014.
3. Aleš Mohorič, Vito Babič, *Fizika 2: učbenik za fiziko v 2. letniku gimnazij in štiriletnih strokovnih šol*, 1. ponatis, Ljubljana, Mladinska knjiga, 2014.
4. Aleš Mohorič, Vito Babič, *Fizika 3: učbenik za fiziko v 3. letniku gimnazij in štiriletnih strokovnih šol*, 1. izd., Ljubljana, Mladinska knjiga, 2014.

## PATENT APPLICATION

1. Denis Arčon, Anton Potočnik, *Method and device for mineral melt stream manipulation*, PCT/SI2014/000068, Slovenian Intellectual Property Office, 26.11.2014.

2. Maja Remškar, Janez Jelenc, Andrej Kržan, *Fluoro-polymer composites with adjusted friction properties*, PCT/SI2014/000052, Slovenian Intellectual Property Office, 19.9.2014.
3. Andraž Rešetič, Jerneja Milavec, Blaž Zupančič, Boštjan Zalar, *Polymer dispersed liquid crystal elastomers (PDLCE)*, GB1404746.8, Intellectual Property Office, 17.3.2014.

## MENTORING

1. Nina Bizjak, *A study of the impact of different bio-chemo-mechanical factors on the course of thrombolysis using optical and magnetic resonance microscopy*: doctoral dissertation, Ljubljana, 2014 (mentor Igor Serša; co-mentor Aleš Blinc).
2. Selestina Gorgieva, *Effect of gelatine scaffolds fabrication as polypropylene mesh coat on implant biocompatibility*: doctoral dissertation, Maribor, 2014 (mentor Vanja Kokol; co-mentor Janez Štrancar).
3. Amid Ranjesh Siahkal, *Stability and metastability of nematic glasses*: doctoral dissertation, Maribor, 2014 (mentor Samo Kralj; co-mentor Milan Ambrožič).
4. Erik Čuk, *Intelligent system for recognition of erythema migrans*: doctoral dissertation, Ljubljana, 2014 (mentor Jurij F. Tasič; co-mentor Matjaž Gams).
5. Simon Jazbec, *Physical properties of dodecagonal quasicrystals, their approximants and comparison with icosahedral and decagonal quasicrystals*: doctoral dissertation, Ljubljana, 2014 (mentor Janez Dolinšek).
6. Jana Milenković, *Computer-aided analysis of soft tissues in medical images*: doctoral dissertation, Ljubljana, 2014 (mentor Jurij F. Tasič).
7. David Seč, *Ordering and local fluids in confined chiral and achiral nematics*: doctoral dissertation, Ljubljana, 2014 (mentor Slobodan Žumer).
8. Donatella Ancora, *UV-vis and <sup>1</sup>H-NMR spectroscopic methods applied to the study of extra-virgin olive oils produced in Tuscany and Apulia*: master's thesis, Pisa, 2014 (mentor Valentina Domenici; co-mentors Tarita Biver, Tomaž Apih).
9. Petra Hohler, *Evaluation of pH dependent photo-physical properties of selected rhodamine derivatives*: master's thesis, Ljubljana, 2014 (mentor Janez Mravljak; co-mentor Stane Pajk).
10. Uroš Jagodič, *Smectic A structure under the influence of forced bend deformation*: master's thesis, Maribor, 2014 (mentor Robert Repnik; co-mentor Samo Kralj).
11. Tadeja Janc, *Chemical glycosylation of rhodamine B and 6G with D-mannose and D-glucose*: master's thesis, Ljubljana, 2014 (mentor Janez Mravljak; co-mentor Stane Pajk).
12. Janez Lužnik, *Magnetic properties of hematite »nano-medusa« nanoparticles*: master's thesis, Ljubljana, 2014 (mentor Janez Dolinšek).
13. Anže Testen, *Effect of albumin on phototoxicity of TiO<sub>2</sub> nanotubes*: master's thesis, Ljubljana, 2014 (mentor Damjana Drobne; co-mentor Tilen Koklič).
14. Katja Vozel, *Study of photoexcited states in new materials for solar cells using pulsed electron paramagnetic resonance*: master's thesis, Ljubljana, 2014 (mentor Denis Arčon).





# 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 to magnetic systems and superconductors. The experimental methods used are suitably diverse, from synthetic chemistry to femtosecond laser spectroscopy. 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 quadruplexes and cilia, and venturing into quantum molecular electronics and nanoelectronics. These and other materials, such as strongly correlated systems, electronically ordered systems and superconductors, were investigated using advanced femtosecond spectroscopy techniques. In many areas we have introduced new materials, technologies and techniques.

Probably the most interesting and far-reaching research in the department in 2014 is related to the discovery of the ultrafast transition to a hidden state in the layered chalcogenide  $1T\text{-TaS}_2$ , published in *Science* in April 2014. This work spawned off a number of new investigations in different directions, which will focus our attention in the forthcoming few years. The mechanism for the observed switching is still rudimentary, and many different aspects still need to be understood and elucidated. The optical switching is of great fundamental interest, because it shows, for the first time, that very stable states can be reached by non-equilibrium non-ergodic methods. Previously, metastability was observed on short timescales, which could not be easily distinguished from simple thermal relaxation. The possibility of achieving electrical switching has led to possible applications, and a significant effort is now devoted to this. A large part of this work was supported by the ERC grant Trajectory.

A number of papers on different aspects of ultrafast phenomena in superconductors and layered chalcogenides have led to a better understanding of the underlying electron dynamics published in *Physical Review B* and the Nature journal *Scientific Reports*. A systematic study of the role of the electron-phonon interaction in cuprate and pnictide superconductors was published in *Physical Review X*.

Experiments on new organic solar cells with the inclusion of MoSI nanowires have led to spectacular increases in efficiency, which is currently being investigated in more detail. The work was published in *Solar Cells*, systematic doping studies of MoSI nanowires led to acceptance of the article for publication in *Nano Letters*.

For the first time we showed the operation of a **field-effect transistor based on  $\text{MoS}_2$  nanotubes**, where previous worldwide efforts have failed. The work represents a milestone in nanodevice physics for our group and in Slovenia, since all the technological steps were performed at the JSI using the facilities of the Nanocenter.

Various polymers composites with MoSI and  $\text{MoS}_2$  have led to interesting developments, reported in *Solar Energy Materials and Solar Cells* and *Journal of Physical Chemistry C: Nanomaterials and Interfaces*.

Important results regarding light and matter interaction, such as the laser-induced generation of periodic polymerisation and improvements in cell calcium detection via fluorescent microscopy were published in *Optics Letters*, *Biochemical and Biophysical Research Communications*, *Liquid Crystals*, and a number of other prestigious journals.

Further studies of magnetic liquid-crystal structures following the report in Nature in 2013 were published in *Soft Matter*, reporting the existence of polar magnetic order, which is a result of the interaction between orientational liquid-crystal ordering and the magnetic order.

## Ultrafast studies of electron dynamics in correlated systems

Hidden states of matter may be created if a system out of equilibrium follows a trajectory to a state that is inaccessible or does not exist under normal equilibrium conditions. We found such a hidden (H) electronic state in a layered dichalcogenide crystal of  $1T\text{-TaS}_2$ , reached as a result of a quench caused by a single 35-femtosecond laser pulse. In comparison to other states of the system, the H state exhibits a large drop of electrical resistance, strongly modified single-particle and collective-mode spectra, and a marked change of optical reflectivity. The H state is stable until a laser pulse, electrical current, or thermal erase procedure is applied, causing it to revert to the



Head:

**Prof. Dragan D. Mihailović**

thermodynamic ground state. We also continued with an investigation of the stability and transport properties of the hidden state in thin  $1T\text{-TaS}_2$  flakes adhered to various substrates by Van der Waals forces to control the substrate-induced strain. The main results were published in *Science* 344, 177 (2014), with the results on the strain effects published separately in *Applied Physics Express* 7, 103201-1, (2014).

Ferromagnetism and superconductivity are antagonistic phenomena. Their coexistence implies either a modulated ferromagnetic order parameter on a length scale shorter than the superconducting coherence length or a weak exchange coupling between the itinerant superconducting electrons and the localized ordered spins. In some iron-based pnictide superconductors the coexistence of ferromagnetism and superconductivity has been clearly demonstrated. The nature of the coexistence, however, remains elusive since no clear understanding of the spin structure in the superconducting state has been reached and the reports on the coupling strength are controversial. We showed in  $\text{Eu}(\text{As,P})_2\text{Fe}_2$ , by a direct optical pump-probe experiment, that the coupling is weak, since the transfer of the excess energy from the itinerant electrons to ordered localized spins is much slower than the electron-phonon relaxation, implying a coexistence without the short-length-scale ferromagnetic order parameter modulation. Remarkably, the polarization analysis of the coherently excited spin wave response points towards a simple ferromagnetic ordering of spins with two distinct types of ferromagnetic domains, as reported in a manuscript accepted for publication in *Scientific Reports* 5, 7754 (2015).

A remarkable change of the quasiparticle relaxation dynamics at the antiferromagnetic transition temperature in iron-based superconductors parent spin-density wave compounds  $A\text{As}_2\text{Fe}_2$ , ( $A=\text{Ba}$ ,  $\text{Sr}$ , and  $\text{Eu}$ ), observed previously using a near-infrared probe, was systematically investigated by broad-band-visible time-resolved spectroscopy. Two different relaxation processes were identified. The behaviour of the slower process, which is strongly sensitive to the magnetostructural transition, was analysed in the framework of the relaxation-bottleneck model involving magnons. The results were also compared to recent time-resolved angular photoemission results and a possible alternative assignment of the slower relaxation to the magnetostructural order parameter relaxation was discussed. The paper was published in *Physical Review B* 89, 165131-1 (2014).

The quasiparticle dynamics with different symmetry was further investigated in the superconducting (SC) and normal states of the high-temperature superconductor  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  ( $\text{Bi}2212$ ) using optical pump-probe experiments with different light polarizations at different doping levels. The observation of distinct selection rules for SC excitations present in A1g and B1g symmetries, and for the pseudogap (PG) excitations present in A1g and B2g symmetries by the probe, and the absence of any dependence on the pump beam polarization leads to the unequivocal conclusion of the existence of a spontaneous spatial symmetry breaking in the PG state not limited to the sample surface. The results were published in *Physical Review B* 90, 094513-1, (2014).

The construction and characterization of a multichannel photodiode detector based on commercially available components with a high signal-to-noise ratio of  $\sim 10^6$  and a rapid frame rate, suitable for time-resolved femtosecond spectroscopy with high repetition femtosecond sources, was presented in a paper published in *Review of Scientific Instruments* 85, 123111-1, (2014).

We used femtosecond optical spectroscopy to systematically measure the primary energy relaxation rate of photoexcited carriers in some cuprate and pnictide superconductors. We found that the rate increases monotonically with increased negative strain in the crystallographic  $a$  axis. Generally, the Bardeen-Shockley deformation potential theorem and, specifically, pressure-induced Raman shifts reported in the literature, suggest that increased negative strain enhances the electron-phonon coupling. The well-known nonmonotonic dependence of the superconducting critical temperature  $T_c$  on the  $a$ -axis strain is also reflected in a systematic dependence  $T_c$  on the relaxation rate, with a distinct maximum at intermediate values ( $\sim 16/\text{ps}$  at room temperature). The empirical nonmonotonic systematic variation of  $T_c$  with the strength of the electron-phonon interaction provides us with a unique insight into the role of electron-phonon interaction in relation to the mechanism of high- $T_c$  superconductivity being a crossover phenomenon, as reported in *Physical Review X* 4, 011056-1, (2014).

We extended previous investigations of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  cuprate superconductors by means of the 3-pulse time-resolved optical spectroscopy technique to different doping levels. The characteristic footprint of the superconducting response was also detected at temperatures above  $T_c$ , indicating the presence of superconducting fluctuations up to 23 K above the  $T_c$ . In classic superconductors an energy gap and phase coherence appear simultaneously with pairing at the transition to the superconducting state. In high-temperature superconductors, the possibility that pairing and phase coherence are distinct and independent processes has led to intense experimental search for their separate manifestations. We showed that it is possible to clearly separate the fluctuation dynamics of the superconducting pairing amplitude from the phase relaxation above the critical transition temperature. Empirically establishing a close correspondence between the superfluid

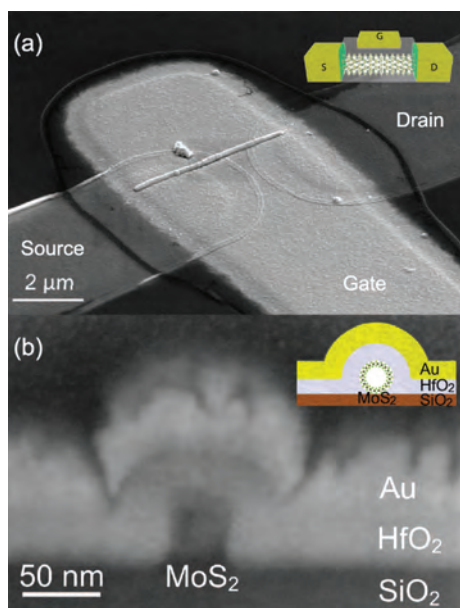


Figure 1: Scanning electron microscope images of a  $\text{MoS}_2$  nanotube field-effect transistor with insets showing schematic representations: a) image of the device and b) image of its cross-section

density measured by THz spectroscopy and superconducting optical pump-probe response over a wide region of temperature, we found that in differently doped  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+d}$  crystals the pairing gap amplitude monotonically extends well beyond the critical temperature, while the phase coherence shows a pronounced power-law divergence at the critical temperature, thus showing that phase coherence and gap formation are distinct processes that occur on different time scales. The results were published in *Scientific Reports* 4, 5656, (2014).

We also presented a detailed analysis of time-resolved optical data on blue bronzes, prototype quasi-one-dimensional charge-density wave (CDW) systems. Numerous coherent (Raman active) modes appear upon the phase transition into the CDW state. We analysed the temperature dependence of the mode frequencies, their damping, as well as their oscillator strengths and phases using the time-dependent Ginzburg-Landau model. We demonstrated that these low-temperature modes are a result of the linear coupling between the Fermi surface nesting driven modulation of the conduction-electron density and the normal-state phonons at the CDW wave vector, and determined their coupling strengths. Moreover, we are able to identify the nature of the excitation of these coupled modes, as well as the nature of the probing mechanisms in this type of experiment. We demonstrated that in incommensurate CDW systems, femtosecond optical excitation initially suppresses the electronic density modulation, while the reflectivity changes at frequencies far above the CDW induced gap in the single-particle excitation spectrum are governed by the modulation of interband transitions caused by lattice motion. This approach can be readily extended to more complex systems with spatially modulated ground states, as reported in *Physical Review B* 89, 045106-1 (2014).

### Theoretical studies on the nanoscale

The theory of electron relaxation in simple metals excited by an ultrashort optical pump is developed on the basis of the solution of the linearized Boltzmann kinetic equation. The kinetic equation includes both the electron-electron and the electron-phonon collision integrals. The widely used, two-temperature model follows from the theory as the limiting case when the thermalization due to the electron-electron collisions is fast with respect to the electron-phonon relaxation. It is demonstrated that the energy relaxation has two consecutive processes. The first and most important step describes the emission of phonons by the photoexcited electrons. It leads to the relaxation of 90% of the energy before the electrons become thermalized among themselves. The second step describes electron-phonon thermalization. The second stage is difficult to observe experimentally because it involves the transfer of only a small amount of energy from the electrons. Therefore, the theory explains why the divergence of the relaxation time at low temperatures has never been observed experimentally. (*Physical Review B* 89, 125102 (2014)).

The theory of the effect of giant dielectric permittivity due to phase separation accompanied by charged inhomogeneities in the low-doped manganites is developed. The effect appears in the vicinity of the second-order magnetic phase transition and is caused by the long-range Coulomb forces. The long-range Coulomb interaction is responsible for the formation of inhomogeneous charged states and determines their characteristic length scales. The phase diagram of the inhomogeneous charged states is derived in the framework of the phenomenological theory of phase transitions. The large value of the static dielectric function reduces the characteristic value of the Coulomb energy of the inhomogeneous state and makes the appearance of the magnetoelectric effect possible. We predict the formation of a state with giant dielectric permittivity and magnetocapacitance effects in that case. (*New Journal of Physics* 16, 073011 (2014)).

### Nanomaterials

One of our fields of study is research on transition-metal chalcogenides and chalcogenides in various low-dimensional forms, in particular nanowires, nanotubes, and nanoflakes.

We have observed the electric field effects on electron transport in multi-walled  $\text{MoS}_2$  nanotubes (NTs) fabricated using a two-step synthesis method from  $\text{Mo}_6\text{S}_9\text{I}_x$  nanowire bundle precursors. The transport properties were measured on 20 single nanotube field-effect transistor (FET) devices, and compared with  $\text{MoS}_2$  layered crystal devices prepared using identical fabrication techniques. The NTs exhibited mobilities of up to  $0.014 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  and an on/off ratio of up to 60. As such, they are comparable with previously reported  $\text{WS}_2$  nanotube FETs, but material defects and imperfections apparently limit their performance compared with multilayer  $\text{MoS}_2$  FETs that have a similar number of layers. We have published this work in *AIP Advances* 4, 097114 (2014).

To improve the functionalization of  $\text{Mo}_6\text{S}_9\text{I}_x$  cluster polymers we have studied the effects of adsorption doping on the electrical transport, aggregation, and optical absorption spectra. Doping results in both enhanced conductivity and aggregated bundles in dispersion. Thanks to this finding,

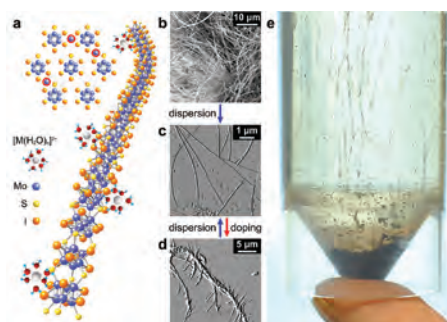


Figure 2: a) Structure of the individual MoSI nanowire and cross-section of a bundle with hexagonal symmetry. Adsorption doping from solution is represented by  $[M(\text{H}_2\text{O})_n]^{2+}$  complexes adsorbed to the side, where M stands for Mg, Ni, or Zn. b-d) Scanning electron microscope and atomic force microscope images of MoSI bundles. e) A photograph of a MoSI nanowire solution, showing aggregation filaments forming upon doping

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**We have built FET transistors using multi-walled  $\text{MoS}_2$  nanotubes.**

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**We have measured the optical spectra of doped MoSI nanowires; spectra of self-doped and adsorption-doped nanowires were compared to the results from femtosecond spectroscopy.**

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**The addition of MoSI nanowires to the active layer of solar cells improves their efficiency.**

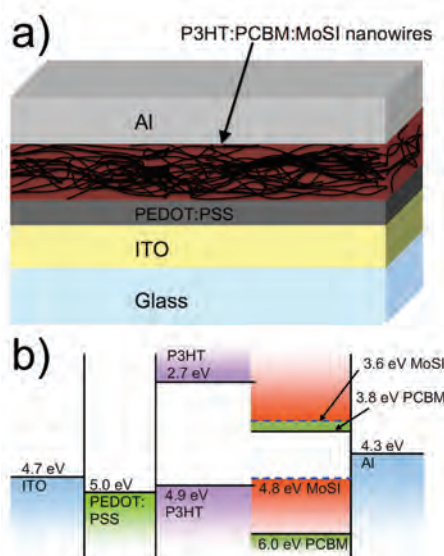


Figure 3: a) Structural scheme of the solar cell b) schematic representation of relevant energy levels of the P3HT:PCBM:MoSI cell

the previously observed different electronic properties of different bundle diameters can be ascribed to self-doping during the synthesis. Doping shifts the characteristic absorption peaks and transfers the oscillator strength to lower energies. Femtosecond optical spectroscopy shows that the spectral signature of adsorption and self-doping indeed originates from the population of electronic levels that are empty or absent in the undoped sample. This work has been accepted for publication in *Nano Letters* in 2015.

By embedding 0.5 wt % highly dispersed  $\text{Mo}_6\text{S}_8\text{I}_x$  molecular wires into the active layer of a bulk heterojunction (polymer:fullerene) solar cell, we could improve the cells' power-conversion efficiency by a factor close to 1.2. We attribute this increase to improved charge transport by the embedded nanowire mesh and envisage a further improvement by using higher nanowire weight fractions and thinner nanowire bundles. This work has been published in *Solar Energy Materials & Solar Cells* 127 (2014) 63–66.

By the extrusion blending of 0.5 wt%  $\text{Mo}_6\text{S}_8\text{I}_x$  molecular wires into polyamide 12 we could increase the Young's modulus by 15%. Differential dynamic calorimetry showed that the nanowires act as a nucleating agent, increasing the crystallization rate and the overall degree of crystallinity of the polyamide, but at the same time the size of the crystals is decreased. This work has been published in *Composites Part B: Engineering* 56, 62–67 (2014).

Recent progress in the exfoliation of layered materials, and the nanofabrication of functional structures, has revived interest in two-dimensional materials with properties complementary to graphene, in particular transition-metal dichalcogenides, such as  $\text{MoS}_2$ . Their potential for electronics has become evident by the realization of a field-effect transistor and a logic-circuit device based on a single monolayer flake.  $\text{MoS}_2$  in its mono- and few-layer form has a significant exciton binding energy of several 100 meV, leading to the consensus that excitons are the primary photoexcited species. Nevertheless, even single layers show a strong photovoltaic effect and work as the active material in high-sensitivity photodetectors, thus indicating efficient charge carrier photogeneration (CPG). By using continuous wave photomodulation spectroscopy we could identify the optical signature of long-lived charge carriers and then study the CPG dynamics with femtosecond pump-probe spectroscopy. We found that the initial photoexcitation yields a branching between the excitons and the charge carriers, followed by excitation-energy-dependent hot exciton dissociation as an additional CPG mechanism. These findings help with the design of more efficient  $\text{MoS}_2$  photovoltaic and photodetector devices. This work is currently under review; a preprint is available at *arXiv:1412.5338*.

We have demonstrated a new, facile method for the controllable synthesis of high-quality single-phase MoN nanowires with a  $T_c$  of 10.5 K from  $\text{Mo}_6\text{S}_8\text{I}_8$  nanowires templates by annealing in flowing ammonia gas at a temperature around 825 °C. The MoN nanowire diameters were controlled exclusively by the  $\text{Mo}_6\text{S}_8\text{I}_8$  nanowires template diameters, which were in the range between several tens and several hundreds of nanometres in this study. Furthermore, we have demonstrated that Ohmic contacts can be prepared on  $\delta_3$ -MoN nanowires with ion-beam-induced platinum deposition using a FIB system, allowing a detailed characterization of the superconducting and transport properties of MoN nanowires. In addition, we have demonstrated the straightforward synthesis of porous  $\delta_3$ -MoN nanowires and nanotubes with nitridation of  $\text{MoS}_2$  nanotubes. X-ray diffraction, scanning electron microscopy with wave dispersive analysis, transmission electron microscopy, four probe electrical transport measurements and SQUID were used to characterize the starting nanowires and nanotubes and the final products. The work was presented in *Nanotechnology* 25, 025601 (2014).

**The addition of MoSI nanowires to polyamide 12 improves its mechanical properties and increases their crystallinity.**

**We have used femtosecond spectroscopy to study the effects of photoexcitation in layers of  $\text{MoS}_2$ , observe the photogeneration of charge carriers and excitons and their dissociation.**

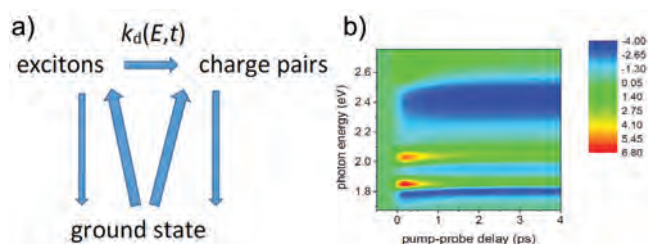


Figure 4: a) Scheme of the photoexcitation dynamics of excitons and charges b) contour plot of the measured transmission spectra in mono- and few-layered flakes of  $\text{MoS}_2$

**We have synthesized  $\delta_3$ -MoN nanowires from MoSI nanowire precursors, measured their transport properties and characterized them.**

**Soft Matter**

We investigated the orientational ordering of inorganic nanotubes ( $\text{MoS}_2$ ) incorporated into a photoreactive liquid-crystalline medium and demonstrated that photopolymerization of the mixture in the orientationally aligned nematic phase leads to plastic composite foils with a profound align-

ment of the nanotubes. The foils exhibit strongly anisotropic mechanical properties. The results were reported in *J. Phys. C* 118, str. 26396 (2014).

In cooperation with TEDA APS at Nankai University (China) we investigated surface-structure modifications of silicon induced by irradiation with a single femtosecond laser pulse and possible application of the resulting surface structures for surface-enhanced Raman scattering. The results were reported in *Optics Letters* 39, p. 343 (2014). Another topic of cooperative investigations was intracellular processes in biological cells. We studied the temperature-induced modifications of radiative activity of fluoropores sensitive to calcium ions. The results were published in *Biochem. Biophys. Res. Commun* 443, p. 888 (2014).

We performed a systematic characterization of the optical diffraction properties of electrically tuneable grating structures based on a combination of polymer and liquid crystals. The grating structure was composed of separated planes of the pure polymer and pure liquid-crystalline material (POLYCRIPS), which was obtained by a two-step fabrication method combining direct laser writing with a subsequent filling of the periodic polymer scaffold with the liquid-crystalline mixture. The results were reported in *Liquid Crystals* 41, p. 1315 (2014).

Cooperative research with Seoul National University (Korea) was focused on investigations of the optical properties of closed-packed arrays of cholesteric liquid crystal droplets. We discovered that colour-selective optical reflection of the droplets provides several interesting possibilities for interdroplet communication processes. This collaborative work was reported in *J. Mater. Chem. C* 2, p. 806 (2014).

We continued with investigations of the surface assembly of guanosine derivatives and guanosine-rich DNA oligonucleotides at the air-water interface and at the surfaces of various solid substrates. We found that lipophilic guanosine derivatives with a single hydrocarbon chain form very robust lamellar complexes that exhibit the characteristics of the nematic liquid crystalline phase. The structural analysis of these lamellar formations was reported in *Colloids Surf. B* 121, p. 114 (2014). In the second half of the year the work was extended to an investigation of effects of various types of cations and anions on the lamellar assembly. We also continued with an analysis of the processes of the formation of G4-DNA wires on solid substrates, which was reported in *Chemistry* 20, p. 3626 (2014).

We have continued studies of the properties of a ferromagnetic phase in suspensions of magnetic platelets in liquid crystals. In this phase, in addition to the orientational order of the liquid crystal, polar magnetic ordering of the platelets is also present, which makes the suspensions also sensitive to magnetic fields, leading to a very large magneto-optic effect. Conversely, the electric field changes the magnetic properties. We have investigated these unique features of the material. They are a consequence of the coupling between the orientational liquid-crystalline and magnetic orders, and we showed that they can be described by a simple macroscopic theory. Moreover, these effects are not only interesting curiosities, but form the basis for possible applications. A detailed study of the static properties was reported in *Soft Matter* 10, 9065 (2014).

### Nonlinear optics

In the Nonlinear Optics Laboratory we study new materials and their interaction with laser light. Integrated optics is a promising technology; however, better materials will increase its potential. In cooperation with North Carolina State University in Raleigh, USA, we study new concepts of compact light sources on the basis of the nonlinear optical conversion of existing lasers into the spectral regions where lasers are not yet available. AlGaIn grown by metalorganic chemical vapour deposition (MOCVD) has a great potential for optoelectronic devices emitting and detecting light in the ultraviolet (UV) wavelength regime.

We study AlGaIn waveguides in various geometries that allow for phase-matched second-harmonic generation and therefore give high efficiency. We study modal dispersion in multimode waveguides and specially prepared waveguides with an alternating sign of the nonlinear coefficient that allows quasi-phase matching.

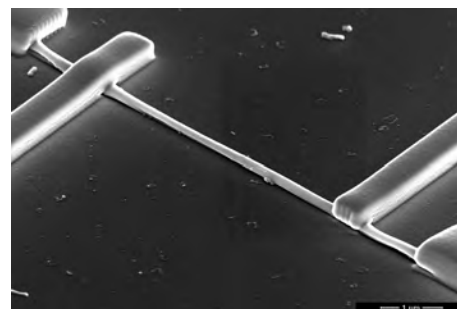


Figure 5: Scanning electron micrograph of the circuit. Electrodes are deposited via ion-beam-induced platinum deposition. The thickness of the electrodes is about  $0.5 \mu\text{m}$ .

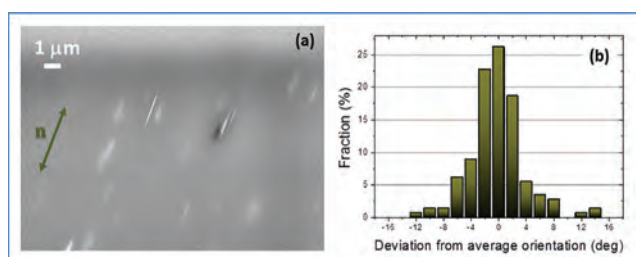


Figure 6: a) SEM depiction of  $\text{MoS}_2$  in photopolymerized liquid crystal b) Orientational division of nanowires

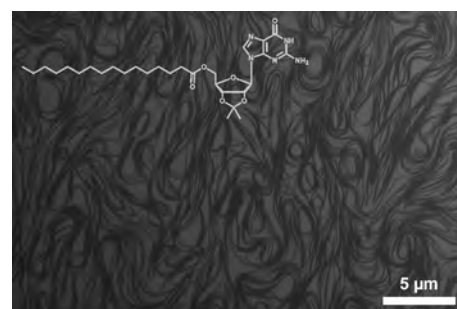


Figure 7: Lamellar Langmuir-Blodgett (LB) structure of a thin film of lipophilic derivative of guanosine transferred from the surface of the water to the  $\text{Si/SiO}_2$  substrate. The picture was taken with an electron microscope

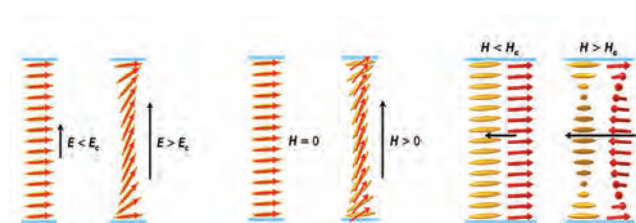


Figure 8: Schematics of converse magnetoelectric, transverse and parallel magneto-optic effects in a ferromagnetic liquid crystal

**We study AlGaIn waveguides in various geometries that allow for phase-matched second-harmonic generation into the UV spectral region.**

### Biomedical optics

We have continued with the development of novel applications based on our custom system for non-contact measurements of laser-induced temperature profiles in biological tissues – pulsed photo-thermal radiometry (PPTR). By combining this experimental technique with a dedicated numerical model of light transport and hemoglobin dynamics in traumatized human skin, we have developed a unique approach for the quantitative assessment of hemoglobin mass diffusion and the physiological degradation rate, as well as the depth of the blood spill in human bruises (hematomas). The obtained knowledge and developed methodology will enable the future development of a protocol for a more accurate and reliable determination of the time of injury in forensic science.

The same experimental technique was also applied to studies of the interaction of strong laser pulses with cutaneous blood vessels in an animal model. We have analysed its suitability for the characterization of the interaction process and/or guidance of dermatologic laser therapy on an individual patient basis. (Collaboration with Beckman Laser Institute, University of California at Irvine.) Both studies were supported by an equipment loan from Fotona, Ljubljana.

We have developed a three-dimensional Monte Carlo (MC) model for light transport in strongly scattering and heterogeneous biological tissues and organs, with rigorous treatment of analytically defined tissue boundaries. In contrast with the common implementation, where tissue boundaries are approximated according to the rectangular

spatial grid, the results of our model do not depend on the positioning or discretization step of the spatial grid.

We have also studied the potential of non-contact tissue characterization using diffuse reflectance spectroscopy (DRS). We have developed an original approach for the rigorous elimination of a known artefact in the measurements of DRS using an integrating sphere. We have analysed the inaccuracy of the DRS analysis using analytical solutions for the transport of light in

strongly scattering tissues, derived within the so-called diffusion approximation. (Collaboration with Norwegian University for Sciences and Technology, Trondheim.)

In addition, we have developed an original procedure that significantly improves the accuracy of such an inverse analysis. The procedure utilizes two comparison runs of a MC numerical model, yet avoids the need to implement and run an inverse MC analysis.

We have participated in the development and characterization of inorganic nanoparticles, which exhibit upconversion fluorescence (UCF), such as  $\text{Yb}^{3+}, \text{Tm}^{3+}:\beta\text{-NaYF}_4$ . Upon further optimization of their optical and chemical properties (biocompatibility), such nanoparticles have great potential for the development of improved techniques for diagnostic imaging and/or the cell-specific therapy of cancer. (Collaboration with Department for Materials Synthesis, IJS)

### Colloidal systems

Studies of colloidal and biomimetic systems were performed in collaboration with the Laboratory of Experimental Soft Matter at the Faculty of Mathematics and Physics, University of Ljubljana. We used magneto-optical tweezers, which were developed and produced in the same laboratory, for studying colloids of different density. Dense colloidal systems were used to study the formation of complex patterns, whereas individual colloidal particles were used to investigate the influence of external fields on their motion. We also developed and optimised photolithographic methods for the fabrication of micrometre-sized particles and microfluidic arrays.

By using a combination of photo and soft lithography we were able to create small particles of different shapes. First, moulds were prepared, which were later filled with a magnetic polymer. Such an approach enables the simultaneous production of a large number of identical superparamagnetic particles (up to  $10^5$  in a single run). Their magneto-responsive behaviour was demonstrated in an experiment with magnetic microgears. We were able to show the transmission of rotation from one magnetically driven microgear to one or several non-magnetic ones. The results of the experiment were published in *RSC Advances*.

Ellipsoidal colloidal particles, also prepared by photolithography, were used to study hydrodynamic interactions in a low-Reynolds-number regime.

It has been shown previously that such elongated particles oscillate when trapped in a strongly focused laser beam of optical tweezers. When two oscillating particles are in the vicinity of each other, the hydrodynamic interactions result in a synchronised motion, similar to beating cilia. We observed the oscillatory motion of ten coupled ellipsoids and observed interesting phenomenon, similar to metachronal waves in cilia. This research is part of doctoral thesis "Beyond hard-walled spherical colloids" by Ivna Kavre.

**We have developed an original approach for the rigorous elimination of the single-beam substitution error (SBSE), an artefact which commonly occurs in measurements of diffuse reflectance spectra using an integrating sphere.**

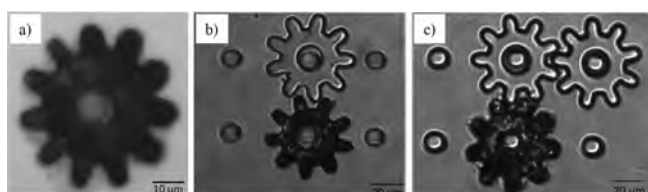


Figure 9: Microgears produced in our laboratory. The dark gears are superparamagnetic and can be driven by an external magnetic field, whereas the light ones are non-magnetic. Rotation of the magnetic field is transferred to the non-magnetic gears. Photo: Ivna Kavre



Successful biomimetic research was continued on the field of artificial swimmers. We created swimmers that were driven externally by a rotating magnetic field and measured their velocities as a function of the field modulation. We were able to prove that their motion is indeed isotropic: different particles move in different directions in the same external field. These detailed and more controlled experiments contributed to the development of an improved theoretical model, which is done in collaboration with the Department of Condensed Matter Physics (F5).

We also closely collaborated with theory groups on dense colloids, studying a two-dimensional system of superparamagnetic particles. Our experimental setup enables the generation of both attractive and repulsive forces between the particles, leading to the formation of different patterns. We concentrated on the regime in which short chains and percolated networks of chains coexist with free colloids. The results of our research appeared in *Langmuir*.

### Some outstanding publications in the past year

1. Stojchevska, L., Vaskivskiy, I., Mertelj, T., Kušar, P., Svetin, D., Brazovskii, S., Mihailović, D.: Ultrafast switching to a stable hidden quantum state in an electronic crystal. *Science*, ISSN 0036-8075, 2014, vol. 344, no. 6180, 177–180, doi: 10.1126/science.1241591. [COBISS.SI-ID 27627303]
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3. Majkić, A., Gadermaier, C., Čelić, N., Topolovek, P., Bratina, G., Mihailović, D.: Mo[<sub>6</sub>S]<sub>(9-x)</sub>I<sub>x</sub> nanowires as additives for enhanced organic solar cell performance. *Solar energy materials and solar cells*, ISSN 0927-0248. [Print ed.], 2014, vol. 127, 63–66. [COBISS.SI-ID 3306491]
4. Tašič, B., Mrzel, A., Huskić, M., Zhang, X., Drevenšek Olenik, I.: Alignment of MoS<sub>2</sub> nanotubes in a photopolymerizable liquid-crystalline material. *The journal of physical chemistry. C, Nanomaterials and interfaces*, ISSN 1932-7447, 2014, vol. 118, iss. 45, 26396–26401, ilustr. <http://pubs.acs.org/doi/abs/10.1021/jp508412w>, doi: 10.1021/jp508412w. [COBISS.SI-ID 2746468]
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6. Mertelj, A., Osterman, N., Lisjak, D., Čopič, M.: Magneto-optic and converse magnetoelectric effects in a ferromagnetic liquid crystal. *Soft matter*, ISSN 1744-683X, 2014, vol. 10, no. 45, 9065–9072, doi:10.1039/C4SM01625D. [COBISS.SI-ID 28078119]
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### Some outstanding publications in the year 2012

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### Organization of conferences, congresses and meetings

1. PIPT5, Photoinduced Phase Transitions and Cooperative Phenomena, Jožef Stefan Institute, Bled, Slovenija, 8–13 June 2014 (organizers)

### Patent granted

1. Ljupka Stojčevska, Tomaž Mertelj, Igor Vaskivskiy, Dragan D. Mihailović, Ultrafast memory by laser quench, SI24265 (A), Urad RS za intelektualno lastnino, 30.6.2014.

## INTERNATIONAL PROJECTS

1. Development of Curved LCD Shutter  
Prof. Martin Čopič  
Kimberly-Clark
2. 7FP - HINTS; Next Generation Hybrid Interfaces for Spintronic Applications  
Prof. Viktor Kabanov  
European Commission
3. 7FP - MoWSeS; Nanoelectronics based on Two-dimensional Dichalcogenides  
Prof. Christoph Gadermaier  
European Commission
4. 7FP - TRAJECTORY, Coherent Trajectories through Symmetry Breaking Transitions  
Prof. Dragan Dragoljub Mihailović  
European Commission
5. Time Resolved Optical Spectroscopy and Manipulation of Electronically Ordered States in Iron Based Superconductors  
Asst. Prof. Tomaž Mertelj  
Slovenian Research Agency
6. Individual Guidance of Medical Laser Treatments Using Photothermal Radiometry  
Prof. Boris Majaron  
Slovenian Research Agency
7. Nonlinear Optical Spectroscopy and Electron Paramagnetic Resonance Study of Valley-polarized Charges in the Monolayer Molybdenum Disulfide  
Prof. Christoph Gadermaier  
Slovenian Research Agency

## RESEARCH PROGRAMS

1. Theoretical Physics of Nuclei, Particles and Fields  
Prof. Sveltana Fajfer
2. Dynamics of Complex Nano-systems  
Prof. Dragan Dragoljub Mihailović
3. Light and Matter  
Prof. Martin Čopič

## R & D GRANTS AND CONTRACTS

1. Cosmology in the Lab - Femtosecond Control of Phase Transitions in Real Time  
Prof. Dragan Dragoljub Mihailović
2. Collective and Molecular Dynamics of Photosensitive Liquid Crystal Elastomers  
Dr. Matija Milanič
3. Optimization Strategies in Biological and Artificial Microfluidic Systems  
Asst. Prof. Andrej Vilfan
4. Thermophoretic Guidance, Accumulation and Sorting of Biomolecules in Microfluidic Devices  
Dr. Natan Osterman
5. Symmetry Breaking in Real Time  
Prof. Dragan Dragoljub Mihailović
6. Center of Competence BioMedical Engineering: CC BME  
Prof. Boris Majaron
7. Development of New Ultrafast Change Memory Devices by Femtosecond Multi-Pulse Spectroscopy (ULTRA-MEM-DEVICE)  
Dr. Ljupka Stojčevska Malbašič
8. COST MP1205; Advances in Optofluidics: Integration of Optical Control and Photonics with Microfluidics  
Dr. Natan Osterman
9. 5th International Conference on Photoinduced Phase Transitions and Cooperative Phenomena - PIP5, Bled, Slovenia, 9-13 June 2014  
Prof. Dragan Dragoljub Mihailović
10. COST MP1302; NanoSpectroscopy  
Prof. Christoph Gadermaier
11. Irradiation and Analysis of Si Samples  
Miloš Borovšak, B. Sc.

## VISITORS FROM ABROAD

1. Dr. Valentin Alek Dediu, CNR-ISMN, Bologna, Italy, 30 March–4 April 2014
2. Prof. Nathalie Kirova-Brazovski, University Paris Sud, Paris, France, 25 May–8 June 2014
3. Prof. Serguei Brazovskii, University Paris Sud, Paris, France, 25 May–8 June 2014
4. Dr. Kenji Kitamura, National Institute for Materials Science, Tsukuba, Ibaraki, Japan, 20–26 June 2014
5. Prof. Martin Fally, Faculty of Physics University, Vienna, Austria, 12–15 June 2014
6. Prof. Stefano Masiero, San Giacomo, Bologna, Italy, 19–21 June 2014
7. Liao Hongyan, TEDA Applied Physics School, Nankai University, Tianjin, China, 22 June–26 July 2014
8. Prof. Roman Yusupov, Kazan Federal University, Lab MRS, Kazan, Russia, 4–17 August 2014
9. Dr. Andrei Shumilin, Ioffe Physical-Technical Institute of the Russian Academy of Sciences, St. Petersburg, Russia, 25 August–30 November 2014
10. Dr. John M. Tranquada, Condensed Matter Physics & Materials Science Department Brookhaven National Laboratory, New York, USA, 29 August 2014
11. Lucian Papazian, Prague City Hall, Prague, Czech Republic, 12–16 September 2014
12. Dr. Bojana Višič, Department of Materials and Interfaces Weizmann Institute of Science, Rehovot, Israel, 21–26 September 2014
13. Lin Lin, School of Physical Science and Technology, Inner Mongolia University, Huhhot, China, 1 October 2014–30 March 2015
14. Dr. Rinat Mamin, Laboratory of Novel Materials, Kazan Physical-Technical Inst. RAS, Kazan, Russia, 17–31 October 2014

## STAFF

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1. Prof. Martin Čopič\*
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  4. Prof. Viktor Kabanov
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  6. Prof. Boris Majaron
  7. Asst. Prof. Alenka Mertelj
  8. Asst. Prof. Tomaž Mertelj
  9. **Prof. Dragan Dragoljub Mihailović, Head**
  10. Dr. Aleš Mrzel
  11. *Dr. Aleš Omerzu, left 01. 03. 14*
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  15. Prof. Marko Zgonik\*
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  17. *Dr. Aleksej Majkič, left 01. 02. 14*
  18. Dr. Matija Milanič
  19. Dr. Andrej Petelin
  20. Dr. Ljupka Stojčevska Malbašič
  21. Dr. Jure Strle
  22. *Dr. Martin Strojnik, left 01. 12. 14*

### Postgraduates

23. Miloš Borovšak, B. Sc.
  24. Tetiana Borzda
  25. Jože Buh, B. Sc.
  26. *Andrej Kovič, B. Sc., left 01. 07. 14*
  27. Andrej Kranjec, B. Sc.
  28. Anna Pogrebna, B. Sc.
  29. Matej Prijatelj, B. Sc.
  30. Peter Topolovšek, B. Sc.
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  33. Luka Vidovič, B. Sc.
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  35. Petra Šutar, B. Sc.
- Technical and administrative staff**
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  37. Janja Milivojevič
  38. Sabina Padežnik, B. Sc.

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# BIBLIOGRAPHY

## ORIGINAL ARTICLE

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  4. Ivan Madan, Janusz Karpinski, Tomaž Mertelj, Dragan Mihailović, "Pump-probe reflectivity study of  $\text{HgBa}[\text{sub}]2\text{CuO}[\text{sub}](4+[\text{delta}])$  cuprate superconductor", In: *Zbornik: 1. del: part 1, 6. študentska konferenca Mednarodne podiplomske šole Jožefa Stefan = 6th Jožef Stefan International Postgraduate School Students' Conference*, 20.-22. 05. 2014, Ljubljana, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2014, pp. 246-254.
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  11. Luka Vidovič, Matija Milanič, Boris Majaron, "Objective fitting of hemoglobin dynamics in traumatic bruises based on temperature depth profiling", In: *Optical Interactions with Tissue and Cells XXV; and Terahertz for Biomedical Applications: February 2-4, 2014, San Francisco, California, United States*, (Progress in biomedical optics and imaging, vol. 15, no. 16), (Proceedings of SPIE, vol. 8941), E. Duco Jansen, ed., Bellingham, SPIE, 2014, pp. 894112-1-894112-9.

## SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK

1. Martina Bačič, Barbara Vilhar, Mojca Vilfan, Simona Strgulc-Krajšek, Cene Fišer, Danilo Bevk, Rok Tkavc, *Spoznavamo naravo 7: učbenik za naravoslovje v 7. razredu osnovne šole*, 1. natis, Kranj, Narava, 2014.
2. Martina Bačič, Barbara Vilhar, Mojca Vilfan, Simona Strgulc-Krajšek, Cene Fišer, Danilo Bevk, Rok Tkavc, *Spoznavamo naravo 7: učbenik za naravoslovje v 7. razredu osnovne šole*, Kranj, Narava, 2014.

## PATENT APPLICATION

1. Adolf Jesih, Andrej Kovič, Aleš Mrzel, *Method for a synthesis of quasi one-dimensional structures of 4D and 5 D (Nb, Mo, Ta, W) transition metals*, EP2723524 (A2), European Patent Office, 30.4.2014.
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## PATENT

1. Ljupka Stojčevska, Tomaž Mertelj, Igor Vaskivskiy, Dragan D. Mihailović, *Ultrafast memory by laser quench*, SI24265 (A), Urad RS za intelektualno lastnino, 30.6.2014.

## MENTORING

1. Andrej Kovič, *Synthesis and characterization of molybdenum based nanowires and nanotubes*: doctoral dissertation, Ljubljana, 2014 (mentor Aleš Mrzel; co-mentor Dragan D. Mihailović).
2. Martin Rigler, *Second harmonic generation in blue and ultraviolet region using AlGaIn waveguides*: doctoral dissertation, Ljubljana, 2014 (mentor Marko Zgonik).





# 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*
- *physics of semiconductors*
- *medical physics*

In the field of reactor physics our research was continued mainly on the development of new methods for the analysis of research and power reactors. A series of experiments were carried out at the TRIGA reactor in collaboration with researchers from CEA – Cadarache in order to determine the reactor kinetic parameters. Measurements at the TRIGA reactor were performed with four fission cells simultaneously and the signals were processed. Thus, we were able to reduce considerably the effect of flux redistribution in the core and improve the procedure to measure the control rod worth with the rod insertion method.

In collaboration with colleagues from CEA - Bruyeres Les Chateles, a plan of a thermal neutron irradiation device was devised and implemented at the TRIGA reactor.

In the framework of the international collaboration coordinated by OECD/NEA we have joined the newly formed working group WPEC SG-41 with the objective of “Improving nuclear data accuracy of  $^{241}\text{Am}$  and  $^{237}\text{Np}$  capture cross-sections”. In 2014, we started with the analysis of the  $^{241}\text{Am}$  cross-section shape in the thermal energy region and its impact on the integral parameters. This work is also consistent with the European project CHANDA.

Reactor Physics Department researchers also provided technical support in 2014 for the safe operation of the Krško nuclear power plant (NPP). We have independently confirmed the nuclear design calculations for the fuel cycle 28. In the framework of the operation “Raziskovalni vavčer” a kinetic evaluation of the NPP Krško core has been performed. As an authorized expert organization in the field of radiation and nuclear safety we have finalized an independent expertise on a NPP Krško reload safety evaluation for the cycle 27 and an expert review of the analysis and testing report for capsule T from the NPP Krško reactor vessel irradiation surveillance program.

We have continued our work on the development of new, and evaluation of the existing, methods of plasma diagnostics with the use of electrostatic probes in the field of plasma physics. This work is done in close collaboration with the University St. Kliment Ohridski from Sofia, and the main effort was put into explaining the behaviour of the Langmuir single and triple probe in the tokamak plasma and the emissive probe in the electronegative plasma. Besides the processing of the data from the tokamaks, we also did experimental work on the Linear magnetized plasma device in our home laboratory. We have also designed and manufactured an ion sensitive probe called the “ball-pen” probe, which will be studied in the future and is starting to be used in tokamaks. In 2014 we have also been actively included into the development of a 2d3v particle-in-cell code for the simulation of the edge plasma of fusion devices in collaboration with TUW (Vienna) and UIBK (Innsbruck). The code should be available for use at the end of 2015. The theoretical and simulation work was directed into a further upgrade of the models of plasma in front of an electron emitting electrode as well as peculiarities in the formation of the potential in front of an electrode with a decisively low voltage drop. We have also started to use our own, upgraded PIC code for simulations of an ion energy analyser. With the help of the BIT1 code we have continued to make simulations of the SOL region of the COMPASS tokamak. We have also continued with various simulations of the formation of the arc inside the gas-discharge tube functioning as a surge protection device on a large scale. Efforts were again also put into studying the plasma double layers, where we have been the first to successfully form an inverted fire-ball inside an magnetized plasma.



Head:

**Asst. Prof. Luka Snoj**



*Figure 1: An inverted fire-ball in the magnetized plasma of the Linear magnetized plasma device in the Laboratory for Plasma Physics in the Reactor Physics Department of the JSI. The grid of the wired-ball is at a higher potential than the surrounding plasma and together with the inter-grid spaces forms an equipotential surface. The electrons in the surrounding plasma see it as a virtual anode, towards which they accelerate and with additional ionization form a new plasma on the inside.*

In the field of **neutron transport calculations for fusion reactors** we continued and expanded our work for JET - Joint European Torus, the largest fusion reactor. Co-workers of the Reactor Physics Division have, in collaboration with the JET staff, performed calculations of the neutron field inside the torus, especially in positions that will be used for the irradiation of samples of structural materials during the upcoming DT campaign. In doing so, we determined the expected damage rate in these materials and the extent of the nuclear heating. The Internal Long Term Irradiation Station of JET has been determined as the position that resembles the closest the conditions expected in ITER. The JSI staff is co-responsible for the maintenance of a model of JET, to be used for transport calculations using the Monte Carlo method. The collaboration with JET takes place within the framework of the new EUROFUSION project under H2020.

The long-term work on the JET g ray camera was expanded within three new projects. We continue to supply the transport calculations for the KN3 camera; in addition, we shifted the focus also to work on a g-ray detector at a distance of more than 10 m from the centre of the torus in the tangential KM6 channel. We also participate in preliminary studies for the analysis of gamma radiation with an energy of 4.4 MeV, originating from materials of the first wall of the torus and comparing its intensity to the g radiation of the same wavelength, originating from  $\alpha$  particle reactions.

In the field of **medical physics** we continued the research focused on positron emission tomography (PET) image analysis, image-guided therapy of cancer and tumour modelling. In part it was a continuation of the existing projects. In the context of the research of fluorothymidine (FLT) uptake stabilization in PET imaging we searched for patterns in the change of the PET image stabilization parameters during radiotherapy, which might help us to understand better the principles of treatment with radiotherapy. The preliminary results show that radiotherapy might have an impact on tumour blood perfusion. We extended the comparison of two PET radiopharmaceuticals (sodium fluoride (NaF) and fluorodeoxyglucose (FDG)), used for the treatment response assessment of bone metastases, to determine the optimal composition of a NaF + FDG cocktail for PET imaging. It was found that the optimal ratio of NaF : FDG is 1:5. Modelling of the tumour response to therapy with the anti-angiogenic drug axitinib was extended with a growth/shrinkage algorithm. It enabled us to reproduce the observed experimental results better; a decrease of the cellular proliferation during the therapy and the rapid rebound of cellular proliferation back to the pre-treatment levels after the cessation of the therapy (proliferative flare). Besides the described projects we also started with a project for the analysis of all the factors that have an impact on the input function (time-dependency of the radiopharmaceutical activity in blood plasma) in dynamic FLT PET imaging. The most interesting finding is that the uncertainties in the measurement of metabolites are of the same order of magnitude as the inter-patient variability, which implicates that these measurements could be equivalently substituted with the population data. For all four projects we obtained clinical data from the University of Wisconsin. Further, and we put a lot of effort into the collaboration with our Slovenian partners (Institute of Oncology, University Medical Centre Ljubljana). We set up two projects with the Institute of Oncology (Radiomic analysis of FDG PET/CT response to therapy in patients with head and neck cancer, similar study in patients with lung cancer) and one with University Medical Centre (assessment of response to therapy by using total bone imaging with FDG PET and flourocholine (FCH)) in patients with metastatic prostate cancer.

### Some outstanding publications in the past year

1. Žerovnik, G., Podvratnik, M., Snoj, L.: On normalization of fluxes and reaction rates in MCNP criticality calculations. *Annals of Nuclear Energy*, ISSN 0306-4549. [Print ed.], 2014, vol. 63, 126–128, doi: 10.1016/j.anucene.2013.07.045
2. Žerovnik, G., Snoj, L., Trkov, A., Barbot, L., Fourmentel, D., Villard, J.-F.: Measurements of thermal power at the TRIGA Mark II reactor in Ljubljana using multiple detectors. *IEEE transactions on nuclear science*, ISSN 0018-9499, 2014, iss. 5, vol. 61, 2527–2531
3. Pigni, M. T., Leal, L. C., Dunn, M. E., Guber, K. H., Trkov, A., Žerovnik, G., Emiliani, F., Kopecky, S., Lampoudis, C., Schillebeeckx, P., Siegler, P.: Evaluation of Tungsten neutron cross sections in the resolved resonance region. *Nuclear data sheets*, ISSN 0090-3752, 2014, vol. 118, 147–150, doi: 10.1016/j.nds.2014.04.022
4. Gilbert, M. R., Dignam, J. J., Armstrong, T. S., Wefel j, S., Blumenthal, D. T., Vogelbaum, M. A., Colman, H., Chakravarti, A., Pugh, S., Won, M., Jeraj, R., Brown, P. D., Jaeckle, K. A., Schiff, D., Stieber, V. W., Brachman, D. G., Werner-Wasik, M., Tremont-Lukats, I. W., Sulman, E. P., Aldape, K. D., Curran, W. J. Jr., Mehta, M. P.: A randomized trial of bevacizumab for newly diagnosed glioblastoma, *N Engl J Med* 370(8), 2014, 699–708
5. Kodeli, I., Zwermann, W.: Evaluation of Uncertainties in  $b_{\text{eff}}$  by Means of Deterministic and Monte Carlo Methods, *Nuclear Data Sheets* 118 (2014), 370–373

6. Fischer, U., Avrigeanu, M., Cabellos, O., Kodeli, I., Koning, A., Leeb, H., Leichtle, D., Rochman, D., Sauvan, P., Sublet, J.-C., Dupont, E., Izquierdo, J., Trkov, A.: The Activities of the European Consortium on Nuclear Data Development and Analysis for Fusion, *Nuclear Data Sheets* 120 (2014), 226–229
7. Leichtle, D., Angelone, M., Batistoni, P., Calderoni, P., Fischer, U., Izquierdo, J., Klix, A., Kodeli, I., Kuc, T., Lilley, S., Majerle, M., Packer, L., Pillon, M., Pohorecki, W., Snoj, L., Villari, R.: The F4E programme on nuclear data validation and nuclear instrumentation techniques for TBM in ITER, *Fusion Engineering and Design* 89 (2014), 2169–2173
8. Chadwick, M. B., Dupont, E., Bauge, E., Blokhin, A., Bouland, O., Capote, R., Carlson, A., Danon, Y., De Saint Jean, C., Forrest, R., Fukahori, T., Ge, Z., Hale, G. M., Herman, M., Ignatyuk, A., Ishikawa, M., Iwamoto, N., Iwamoto, O., Jandel, M., Jacqmin, R., Kawano, T., Kunieda, S., Kahler, A., Kodeli, I., Koning, A., Leal, L., Lee, Y.O., Lestone, J., Lubitz, C., MacInnes, M., Moxon, M., Noguerra, G., Palmiotti, G., Plompen, A., Pritychenko, B., Pronyaev, V., Rochman, D., Romain, P., Roubtsov, D., Schillebeeckx, P., Simakov, S., Sublet, J. C., Talou, P., Thompson, I., Trkov, A., Vogt, R., van der Marck, S.: The CIELO Collaboration: Neutron Reactions on  $^1\text{H}$ ,  $^{16}\text{O}$ ,  $^{56}\text{Fe}$ ,  $^{235,238}\text{U}$ , and  $^{239}\text{Pu}$ , *Nuclear Data Sheets* 118 (2014), 1–25
9. Salvatores, M., Palmiotti, G., Aliberti, G., Archier, P., De Saint Jean, C., Dupont, E., Herman, M., Ishikawa, M., Ivanova, T., Ivanov, E., Kim, S. J., Kodeli, I., Manturov, G., Mcknight, R., Pelloni, S., Perfetti, C., Plompen, A., Rearden, B. T., Rochman, D., Sugino, K., Trkov, A., Wang, W., Wu, H., Yang, W. S.: Methods and Issues for the Combined Use of Integral Experiments and Covariance Data: Results of a NEA International Collaborative Study, *Nuclear Data Sheets* 118 (2014), 38–71
10. Kodeli, I., Milocco, A., Ortego, P., Sartori, E.: 20 Years of SINBAD (Shielding Integral Benchmark Archive and Database), *Progress in Nuclear Science and Technology*, Volume 4 (2014), 308–311

## INTERNATIONAL PROJECTS

1. Advisory Services for the Independent Evaluation of Root Cause Analysis for Six Leaking Fuel Assemblies - Krško Cycle 26  
Dr. Marjan Kromar  
NAC International, Inc.
2. F4E-FPA-168-01; Nuclear Data Improvements and Development of Tools - Nuclear Data Evaluation  
Prof. Ivan Aleksander Kodeli  
European Commission
3. Specific Grant Agreement; Cu Experiment and TBM Nuclear Instrumentation  
Prof. Ivan Aleksander Kodeli  
European Commission
4. 7FP - CHANDA; Solving CHALLENGES in Nuclear DATA  
Prof. Ivan Aleksander Kodeli  
European Commission
5. F4E-GRT-168.02; Specific Grant Agreement: Nuclear Data Improvements and Development of Tools - Nuclear Data Evaluation  
Prof. Ivan Aleksander Kodeli  
European Commission
6. Feasibility Study and Installation of Thermal Neutron Driven 14 MeV Neutron Converter into the TRIGA Research Reactor  
Asst. Prof. Luka Snoj  
IAEA - International Atomic Energy Agency
7. Integral Measurements for the Validation of the Dosimetry Cross Sections; F41031 Testing and Improving the IAEA International Dosimetry Library for Fission and Fusion (IRDF)  
Dr. Gašper Žerovnik  
IAEA - International Atomic Energy Agency
8. Experimental Verification of Kinetic Parameters of the TRIGA Reactor and Upgrade of the Digital Meter of Reactivity  
Dr. Igor Lengar  
Slovenian Research Agency
9. Experimental Verification of Neutron Flux Form Factors and Qualification of a New Wide Range Multichannel Neutron Instrumentation  
Dr. Gašper Žerovnik  
Slovenian Research Agency
10. Design of Irradiation Device for FT-TIMS Method at the JSI TRIGA Mark II Reactor  
Asst. Prof. Luka Snoj  
Slovenian Research Agency
11. Neutron Transport in Fusion and Fission Reactors by Coupling of Deterministic and Monte Carlo Methods  
Dr. Igor Lengar  
Slovenian Research Agency
12. Development and Application of Kinetic Analysis for PET for Optimization of Antiangiogenic Targeted Cancer Therapies  
Prof. Robert Jeraj  
Slovenian Research Agency
13. OECD/Nuclear Energy Agency

- Prof. Ivan Aleksander Kodeli  
Slovenian Research Agency
14. RU-FU, EUROFUSION; Research Unit - Administration and Services  
Asst. Prof. Luka Snoj  
European Commission
  15. Enabling Research-2-FU, EUROFUSION  
Dr. Jernej Kovačič  
European Commission
  16. Exploitation of DT Operation for ITER-JET3-FU, EUROFUSION  
Asst. Prof. Luka Snoj  
European Commission
  17. Education-ED-FU, EUROFUSION  
Asst. Prof. Luka Snoj  
European Commission
  18. PMU-International Collaboration, EUROFUSION  
Prof. Ivan Aleksander Kodeli  
European Commission
  19. JET Enhancements-JET4-FU, EUROFUSION  
Dr. Igor Lengar  
European Commission

## RESEARCH PROGRAM

1. Reactor Physics  
Asst. Prof. Andrej Trkov

## R & D GRANTS AND CONTRACTS

1. Neutron Calculations for Use with Neutron Diagnostics - Application to the JET Fusion Reactor  
Dr. Igor Lengar
2. Development of Methodology for Calibration of Neutron Detectors with a 14.1 MeV Neutron Generator - JET Fusion Reactor Case  
Asst. Prof. Luka Snoj
3. Analysis of Material Damage and Activation in Large Scale Fusion Reactors - Application to the Reactor JET  
Dr. Igor Lengar
4. Determination of Computational Framework for Treating Gas Discharges in Case of Surge Protection Gas Discharge Tubes  
Dr. Jernej Kovačič
5. Irradiation and Analysis of Si Samples  
Asst. Prof. Andrej Trkov



## NEW CONTRACTS

1. Reload Operational Core Analysis, Post Refueling Nuclear Design Check Tests, PIS and KFSS cycle Specific Data for Future Fuel Cycles  
Dr. Marjan Kromar  
Krško Nuclear Power Plant
2. Expert Review of the Analysis and Testing Report for Capsule T for the Krško Reactor Vessel Irradiation Surveillance Program  
Dr. Marjan Kromar  
Krško Nuclear Power Plant
3. Expert Review of the Document Reload Safety Evaluation (RSE) of Cycle 27  
Dr. Marjan Kromar  
Krško Nuclear Power Plant
4. Development of Advanced Methods for the Description of Dynamic Processes in a Nuclear Reactor  
Asst. Prof. Luka Snoj  
Krško Nuclear Power Plant

## VISITORS FROM ABROAD

1. Prof. Tsviatko K. Popov, Faculty of Physics, University St. Kliment Ohridski, Sofia, Bulgaria, 8–22 February 2014
2. Dr. Steven Van Dyck, SCK CEN, Nuclear Materials Science, Mol, Belgium, 6–10 January 2014
3. Dr. Jonathan S. Morrell, Y-12 National Security Complex, Oak Ridge, TN, USA, 6–10 January 2014
4. Dr. Jean Christophe Sublet, Culham Centre for Fusion Energy – CCFE, Abingdon, Oxfordshire, United Kingdom, 4–6 March 2014
5. Embie Hasan, Faculty of Physics, University St. Kliment Ohridski, Sofia, Bulgaria, 5 May–2 June 2014
6. Anne-Laure Faure and Anne-Claire Pottin, CEA, Cadarache, France, 23–24 June 2014
7. Dr. Loic Barbot, CEA, Cadarache, France, 30 June–11 July 2014
8. Dr. Damien Fourmentel, CEA, Cadarache, France, 30 June–11 July 2014
9. Mr. Fausto Franchescini, Westinghouse, Cranberry Township, Pennsylvania, USA, 8–11 September 2014
10. Mr. Niklas Barringer, ISEC, Höganas, Sweden and Miroslav Gregorič, MSc., International Atomic Energy Agency, Vienna, Austria, 9 December 2014

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# DEPARTMENT OF EXPERIMENTAL PARTICLE PHYSICS

# F-9

*Departmental research is devoted to experimental studies of elementary particles, to reveal the ultimate building blocks of matter and the nature of the interactions between them. Experiments are carried out within large collaborative programmes at international centres for particle physics at CERN near Geneva and at KEK in Tsukuba. The department is also engaged in developing and applying the technologically advanced particle detectors that are demanded by such measurements. Astroparticle physics is an emerging field applying experimental techniques of particle physics to solve astrophysical problems. Slovenian researchers are participating in measurements of ultra-high-energy cosmic rays with the Pierre Auger observatory, spread over a surface of 3000 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 only affordable as joint international enterprises. Thus, future accelerators will be unique facilities of their kind, the first being the Large Hadron Collider (LHC), just completed at the European Organization for Nuclear Research (CERN) near Geneva. Researchers will exploit this facility to perform experiments in presently inaccessible regions of energy, which, though pushed higher and higher, still remains minute compared to that of the vast blast of the Big Bang that led to the creation of the Universe.

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

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

In the field of astroparticle physics we are part of the Pierre Auger collaboration (250 researchers, 94 institutions from 17 countries), which uses a giant scale (3000 km<sup>2</sup>) observatory near Malargue in Argentina for the detection of ultra-high-energy cosmic rays. This endeavour is carried out in collaboration with colleagues from the University of Nova Gorica.

A more detailed report on the activities of 2014 follows, focused on the contributions of our researchers:

## ATLAS experiment

The volume and quality of data delivered by the Large Hadron Collider LHC at CERN in 2011 and 2012 exceeded the most optimistic expectations and the data analysis has been occupying the scientists of the ATLAS collaboration throughout 2013 and 2014. In addition to the analysis of existing data, the collaboration is preparing for the re-start of the Large Hadron Collider LHC in 2015, when it will begin to operate at an unprecedented center-of-mass energy of 13 TeV.

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

The most visible analyses of the ATLAS collaboration were the ones determining the properties of the Higgs (Brout-Englert-Higgs), discovered by the ATLAS and CMS collaborations in July 2012. For its theoretical prediction, the Nobel Prize for Physics in 2013 was given to P. Higgs and F. Englert and



Head:  
**Prof. Marko Mikuž**

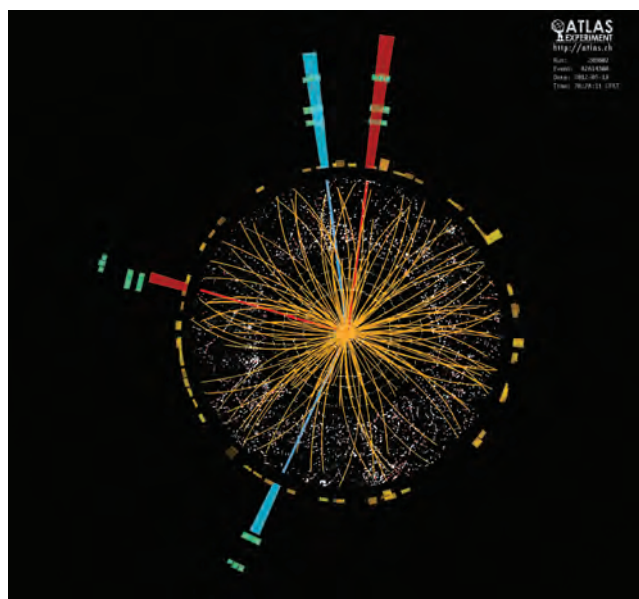


Figure 1: Event display of a  $H \rightarrow 4$  lepton candidate event with  $m(4l) = 124.5$  GeV without Z mass constraint. The masses of the lepton pairs are 70.6 GeV and 44.7 GeV. The tracks and clusters of the two electron pairs are coloured red and blue, respectively.

**Searches for beyond-Standard-Model physics continued throughout 2014, and while a plethora of possible theories were statistically excluded, no discoveries of New Physics were made as yet. There are, however, good indications that such discoveries could be made when the LHC restarts in 2015 at even higher energies.**



Figure 2: Installation of Diamond beam monitor (DBM) on the support structure of pixel detector. It will provide complementary luminosity measurement to the BCM

the prize itself cites the discovery of the Higgs boson by the ATLAS and CMS collaborations. This result is an important advance in our understanding of the basic forces holding the Universe together. Searches for beyond-Standard-Model physics continued throughout 2014 and while a plethora of possible theories were statistically excluded, no discoveries of New Physics were made as yet. There are, however, good indications that such discoveries could be made when the LHC restarts in 2015 at the even higher energies. In 2014 the ATLAS collaboration published more than 80 scientific papers in the most distinguished scientific journals [1], bringing the total number of scientific papers published by the collaboration to 353, with more than a hundred further papers in preparation.

The Slovenian group took a leading role in designing, building and operating the ATLAS Beam Condition Monitor (BCM), Beam Loss Monitor (BLM), Radiation Monitor (RADMON) and Diamond Beam Monitor (DBM). The BCM was built to monitor conditions of the LHC beams and issue warnings about unexpected and potentially dangerous situations. Before shutdown it acted as the ATLAS main luminosity monitor, reporting a great majority of almost  $30 \text{ fb}^{-1}$  that were delivered to ATLAS. The BLM, on the other hand, acted as a safety system and protected the ATLAS Inner Detector from potential damage

by LHC beams, which fired and extracted LHC beams twice in summer 2011. RADMON records the doses received by different parts of the ATLAS Inner Detector. A newly built DBM was installed during the shutdown and will be used for the first time in 2015. It is built from a pCVD diamond sensor and pixel readout chip with pixels of size  $250 \mu\text{m} \times 50 \mu\text{m}$ . It will provide complementary luminosity measurement to the BCM.

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

The Belle detector finished taking data in 2010, allowing time for the upgrade of the detector – Belle II. The latter will start taking data in 2017. In parallel with the Belle II construction still a number of measurements performed on Belle data set are ongoing. The main aim of the measurements is the identification of so-far unknown particles and processes, which one usually addresses as New Physics (NP). These are – among others – responsible for a total prevailing of matter (particles) over antimatter (antiparticles) in the Universe.

**The Belle collaboration performed a number of precision measurements significantly constraining possible values of the parameters of the models of New Physics. The construction of the Belle II detector including the sub-detector modules for particle identification based on Cherenkov radiation and semiconductor pixel modules is well under way.**

In 2014 researchers of the Belle international collaboration (472 researchers from 80 institutions and 18 countries) achieved several important scientific results. In the field of the so-called exotic particles (particles that according to their properties cannot be categorized in the standard classification of heavy particles – hadrons), started back in 2003 with the Belle discovery of the  $X(3872)$  particle (the journal paper with this result already has more than 1000 citations), the LHCb collaboration at the LHC collider finally confirmed the existence of the electrically charged exotic particle  $Z(4430)^+$  first observed by the Belle experiment. This was followed by the experimental observation of another exotic particle  $Z(4200)^-$ . This field of research promises to provide a new insight into the nature of the strong nuclear force, which is also responsible for bounding protons and neutrons inside the nuclei.

A new precise measurement of neutral B meson decays,  $B^0 \rightarrow \pi^0 \pi^0$ , has also been performed [2]. Knowledge of the decay rate of this rare decay mode (around 1 in a million of  $B^0$  mesons decays through this decay) will shed light on one of the discrepancies between the predictions of theory and the experimental measurements, which may be due to the effects of NP.

A similar situation is true for the measurement of  $B \rightarrow \tau \gamma$  decays. These decays represent an experimental challenge due to the presence of two or more neutrinos in the final state that are not detected by the detector. Members of the Belle collaboration developed a method that enables the reconstruction of such decays and their isolation from the background processes.

In 2014 researchers at the BaBar experiment at SLAC in the USA and at the Belle experiment jointly published a monograph (Fig. 3) summarizing and detailing a decade of measurements in the field of B meson physics

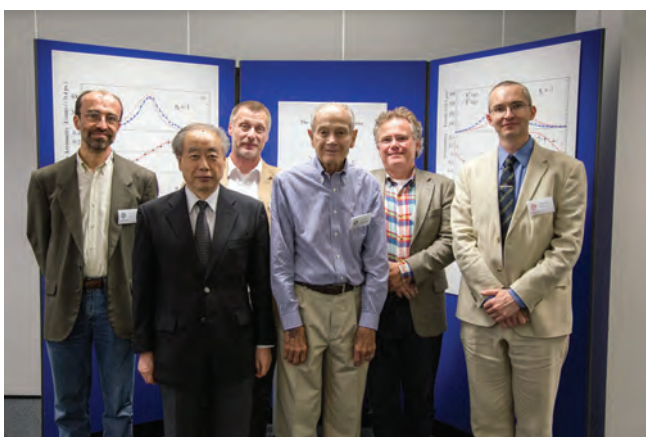


Figure 3: The Physics of the B Factories monograph editors (from left in rear row: B. Yabsley, B. Golob, Th. Mannel in A.J. Bevan) with Nobel Prize laureates M. Kobayashi (left in front row) and J. Cronin during the promotion of the book in London.



with a description of the measurement methods, the results and their interpretations [3].

In the construction of the Belle II detector members of the collaboration (604 researchers from 96 institutions and 23 countries) achieved several milestones. The construction of the Central Drift Chamber, including more than 14000 sense wires, was finalized.

After specification tests orders for the mass production of all the quartz plates needed in one of the most delicate parts of the detector – the iTOP detector – were placed. This detector module serves for charged particle identification through the detection of the Cherenkov light emitted by particles traversing the quartz. All 18 individual modules (Fig. 4) are expected to be finalized in December 2015.

In the production of the pixel detector modules based on the newest DEPFET (DEPLETED Field Effect Transistor) technology the most demanding production step, the metallization process, has been fixed based on results of the tests. The pixel sub-detector will enable a determination of the decay vertices of short-lived particles with an accuracy of 50  $\mu\text{m}$ . After this step the mass production of the pixel detector modules will start.



Figure 4: Preparation of quartz modules for charged particle identification through the detection of the Cherenkov light in BELLE spectrometer

### Pierre Auger observatory

The Earth is exposed to a permanent rain of cosmic particles from outer space. Most of the particles are fully ionized atomic nuclei, moving with relativistic energies. The bulk of them with energies up to 1017 eV originate within our Milky Way. Some particles have a thousand-times-higher energies, i.e., around  $10^{20}$  eV. To clarify the origin of the highest-energy particles, their properties like energy, arrival direction and the particle type (photons, protons, atomic nuclei) have to be measured. The highest-energy cosmic rays are extremely rare. On earth, one particle is registered in an area of 100 square kilometres in a hundred years. The measurement of such particles requires a huge measurement device that is operated for a long time.

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

The advent of the Pierre Auger Observatory has dramatically advanced our understanding of ultra-high-energy cosmic rays (UHECRs). A strong flux suppression at the highest energies, similar to the one expected from cosmic-ray energy losses in the CMB (GZK-effect), has been observed beyond any doubt. Moreover, strong flux limits have been placed on the photon and neutrino components at EeV energies disfavoring exotic particle physics models for the origin of the most energetic cosmic rays. Finally, indications are found for the presence of a large-scale anisotropy, both below and above the energy of the ankle, and for an anisotropy on smaller angular scales at  $E > 5.5 \cdot 10^{19}$  eV.

The all-particle cosmic ray energy spectrum carries combined information about the UHECR sources and about the galactic and/or intergalactic media through which the cosmic rays propagate. The flux suppression due to energy losses by photo-pion production and photodisintegration in the CMB (GZK-effect) is the only firm prediction ever made concerning the shape of the UHECR spectrum. First observations of a cut-off were reported by Auger. However, at present, we cannot be sure whether this flux suppression is an imprint of the aforementioned GZK energy losses or whether it is related to the maximum cosmic ray acceleration energy at the sources. Despite the high level of precision reached, the all-particle energy spectrum by itself does not allow one to conclude unambiguously about the origin of the spectral structures and thereby about the origin of cosmic rays from the ankle to the highest energies. Additional key information is obtained from the mass composition of cosmic rays. Unfortunately, the measurement of the primary masses relies on comparisons of data to extensive air shower (EAS) simulations with the latter serving as a reference. EAS simulations, however, are subject to uncertainties mostly

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**The Auger Observatory has collected 10 years of data, six of which were with the fully instrumented observatory. The results obtained so far have dramatically advanced our understanding of ultra-high-energy cosmic rays.**

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because hadronic interaction models need to be employed at energy ranges much beyond those accessible to man-made particle accelerators. Therefore, the advent of LHC data, particularly those measured in the extreme forward region of the collisions, is of great importance to cosmic-ray and air-shower physics and have already helped to tune the hadronic interaction models. The data from the Pierre Auger Observatory suggest an increasingly heavier mass composition above  $4 \cdot 10^{18}$  eV when compared to post-LHC interaction models. These data complement those of the energy spectrum in a remarkable way: the change of the composition starts just above the ankle and the composition becomes increasingly heavy towards the flux-suppression region, which is exactly the behaviour expected from the maximum energy scenario.

Further important information about the nature and origin of UHECR is contained in the distribution of their arrival directions over the sky. Unlike energies or primary mass, the arrival directions of cosmic-ray events are practically free from systematic errors. Apart from the (unknown) distribution of sources over the sky, the

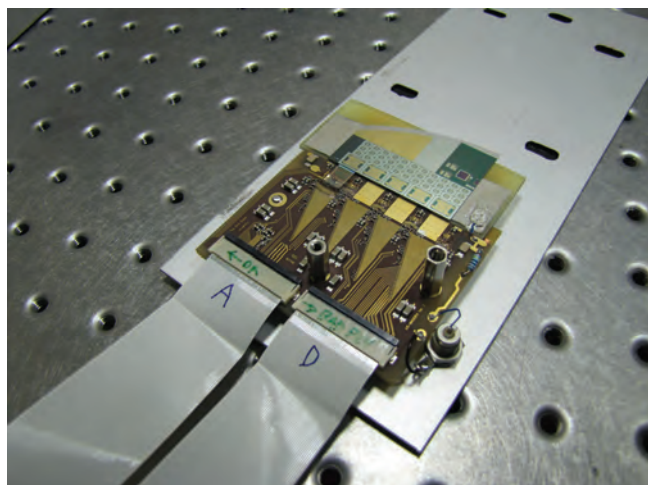


Figure 5: The printed circuit board (PCB) and application-specific integrated circuit (ASIC) are connected via thin, 20 micrometres aluminium wire bonds. For operation in a magnetic field, the wires must be encapsulated.

two main factors that determine the UHECR anisotropy are deflections in cosmic magnetic fields and attenuation due to the interactions with the background radiations. The Pierre Auger Collaboration has performed a number of anisotropy searches on different angular scales and by applying different techniques. No significant deviations from isotropic expectations were found throughout the analyses performed, which provides constraints on the production of cosmic rays above  $10^{18}$  eV if they were emitted from stationary galactic sources densely distributed in the galactic disk. At high energies (around and above the cut-off in the spectrum) the situation is more interesting. The Auger collaboration has reported an excess of UHECR events with  $E > 55$  EeV around the direction towards the Centaurus supercluster at a distance of about 60 Mpc and Centaurus A, a close AGN at a distance of about 3.5 Mpc. The largest excess was found for a circular region of the angular size  $18^\circ$ . This region includes 10 out of 60 events above 55 EeV in the data set of this analysis, while 2.44 are expected from isotropy.

The Auger Observatory has collected 10 years of data, six of which were with the fully instrumented observatory. The results obtained so far have dramatically advanced our understanding of ultra-high-energy cosmic rays. However, despite more than 40,000  $\text{km}^2\text{sr yr}$  of high-quality data being analysed, it is still not possible to determine whether the observed flux

suppression is due to the GZK-effect or due to the limiting acceleration power of the sources. It is evident that this puzzle must be resolved in order to identify the sources or source regions. The key lies in a better identification of the primary composition, especially extending to the highest energies. The most promising way to obtain further composition-sensitive information is the discrimination between the electromagnetic and muonic components of the shower with ground-array measurements. Intense R&D efforts have thus been started in this direction and five different options for complementing the surface detector array have been investigated. They include placing scintillators or resistive plate chambers with a pad readout beneath the tanks or into the ground, placing scintillators on top of the tanks, or segmenting the existing water Cherenkov detectors into a top and bottom layer. The principle is always the same: the top detector samples more of the electromagnetic component, while the response of the bottom detector becomes more pronounced to muons.

The different technical realizations have been assessed under considerations of performance, technical complexity, robustness, deployment, and costs with the result that the scintillators to be placed on top of the tanks were given priority for realization. The detector will be further optimized and new surface detector electronics be produced to facilitate the readout of the extra channels and to provide more powerful triggers and better monitoring. Another small PMT to be placed into the water Cherenkov tank is considered for increasing the dynamic range of the detector stations, enabling us to measure signals more closely to the shower core than has been possible up to now. If funding is provided, R&D and prototyping would terminate at the end of 2015 and construction could start in 2016 and last for about two years. The upgraded observatory would then take data into 2023, thereby doubling the statistics that have been collected with the present setup. Data taking would continue uninterrupted during this period, as only new detectors will be added.

#### Distributed computing

The SiNET Tier-2 distributed computing site has increased its capacity to 4200 cores and 2500 TB of data-storage space in 2014. In addition, a dedicated 10 Gb/s network link was established to increase the throughput to NDGF Tier-1. The centre was integrated into the LHCONE network to optimize the data flow between the grid sites. 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. The Slovenian distributed infrastructure incorporates seven clusters from the Jožef Stefan Institute, Arnes, Acurt, University of Nova Gorica, and several others are in the process of joining with a vision to create a powerful distributed computing infrastructure in Slovenia. The SiGNET is a full member of the international organizations EGI/InSPIRE, wLCG and Nordugrid and had participated in several joint projects related to support, maintenance and planning of the computing infrastructure as well as the development, distribution and deployment of the distributed computing infrastructure. It participated in education at several distributed computing workshops organized at Arnes and the Jožef Stefan Institute. The main objective of SiGNET Tier-2 is to support the data processing and storage for the international experiments ATLAS, Belle, Belle 2, and Pierre Auger. In addition, the site provides support to Slovenian research and educational organizations. Within the ATLAS collaboration, we have been working on the integration of the European and Asian supercomputer centres (HPC) in wLCG.

### Detector development

Modern diagnostic imaging is driven towards combinations of complementary imaging modalities. At the Jožef Stefan Institute we tested the compatibility of PET imaging technology with silicon sensors and magnetic resonance imaging (MR). To this end, the imaging module portrayed in the figure was built, composed of evaluation silicon sensor sensitive to photons used in PET and SPECT connected to electronics insensitive to magnetic fields used in MR. The printed circuit board (PCB) and application-specific integrated circuit (ASIC) realized on a silicon chip are connect via thin, 20-micrometres aluminium wire bonds (Fig 5). For the operation in the magnetic field, the wires must be encapsulated in glue, to prevent bond tearing due to magnetic forces driven by switching signal currents. At the Institute we have developed a glue applicator able to handle the thin wires spaced at intervals below 200 micrometres, which maintains the circuit functionality. The circuits were successfully tested at the Laboratory for Magnetic Resonance Imaging of the Jožef Stefan Institute.

The development of radiation hard silicon detectors is very important for future high-energy experiments. We used the innovative edge-TCT method, developed at our laboratory, to measure the electric field in CMOS silicon detectors. The detectors were irradiated at the nuclear reactor in Podgorica near Ljubljana with neutrons up to fluences of  $5 \times 10^{14} \text{ cm}^{-2}$ . The CMOS sensors are serious candidate to replace conventional silicon detectors. They offer on-chip first-stage processing of a signal at a lower price.

We performed more than 120 irradiations at Nuclear Reactor Podgorica in the framework of AIDA (Advanced European Infrastructures or Detectors at Accelerators) for 12 interested institutions. In the past year of this project the emphasis was on upgrades for the ATLAS, CMS and BELLE detectors.

### Awards and appointments

1. Tara Nanut: Honorary document for the students with the best study performance (Svečana listina za študente Univerze v Ljubljani za najboljši študijski uspeh), University of Ljubljana, Ljubljana, Slovenia.

## INTERNATIONAL PROJECTS

- |  |  |
|--|--|
| 1. Design, Procurement and QA of Flex-Rigid Hybrids<br>Prof. Marko Mikuž<br>European Organization for Nuclear Research   | Hadrons at the Belle II Experiment<br>Prof. Boštjan Golob<br>Slovenian Research Agency   |
| 2. Irradiations in TRIGA Nuclear Reactor<br>Prof. Vladimir Cindro<br>European Organization for Nuclear Research  | 9. Evaluation of the Prototype of a Double-ring PET Device<br>Prof. Marko Mikuž<br>Slovenian Research Agency                                     |
| 3. 7FP - EGI-InSPIRE; European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe<br>Prof. Marko Mikuž<br>European Commission | 10. Study of Silicon Detectors and Structures by using Scanning Transient Current Tecnique<br>Dr. Gregor Kramberger<br>Slovenian Research Agency |
| 4. 7FP - AIDA; Advanced European Infrastructures for Detectors at Accelerators<br>Prof. Marko Mikuž<br>European Commission   |  |
| 5. 7FP - HadronPhysics3; Study of Strongly Interacting Matter<br>Prof. Samo Korpar<br>European Commission  |  |
| 6. FERRO-PATCH; Frequency and Polarisation Agile Microstrip Patch Antenna based on Ferrelectric Varactors<br>Prof. Vladimir Cindro<br>ESA/ESTEC.                         |  |
| 7. Development and Tests of a Method for Particle Identification with a TOP Counter<br>Prof. Marko Starič<br>Slovenian Research Agency                                   |  |
| 8. Methods and Accuracies of the Mixing and CP Violation Measurements of the Charmed   |  |

## RESEARCH PROGRAMS

1. Astroparticle Physics  
Prof. Marko Zavrtanik
2. Experimental Particle Physics  
Prof. Marko Mikuž

## R & D GRANTS AND CONTRACTS

1. Development of Solid State Detectors for Particle Physics Experiments  
Prof. Vladimir Cindro

2. Novel Detection Methods based on Cherenkov Radiation  
Prof. Peter Križan
3. ATLAS Diamond Beam Monitor  
Prof. Marko Mikuž
4. Search for Microscopic Black Hole Signatures with Ultra-high Energy Cosmic Rays  
Prof. Marko Zavrtanik
5. Novel Scintillation Detectors for Precision Particle Physics Experiments  
Prof. Peter Križan
6. Development of In-vivo Dosimetry for Applications in Radiotherapy  
Dr. Gregor Kramberger
7. Collaboration ATLAS  
Prof. Marko Mikuž
8. Collaboration CERN RD-39  
Prof. Marko Mikuž
9. Collaboration CERN RD-42  
Prof. Marko Mikuž
10. Collaboration CERN RD-50  
Prof. Marko Mikuž
11. Collaborations Belle in Belle II  
Prof. Peter Križan
12. Collaboration CIMA; Cameras for Imaging in Medical Applications  
Prof. Marko Mikuž

## NEW CONTRACTS

1. Reliability Investigation of High Density Interconnect Circuits  
Prof. Vladimir Cindro  
Intec TIV, d. o. o.
2. HPC Puppet  
Prof. Andrej Filipič  
Arctur, d. o. o.

## VISITORS FROM ABROAD

1. Prof. Peter Jenni, University of Freiburg & CERN, Germany & Switzerland 13–15 January 2014
2. Prof. Masanori Yamauchi, Institute of Nuclear & Particle Studies, KEK, Tsukuba, Japan, 3 September 2014
3. Dr. Silvio Sciortino, Department of Physics and Institute for Nuclear Physics (INFN), Florence, Italy, 9–11 September 2014
4. Prof. Toru Iijima, University of Nagoya, Nagoya, Japan, 14–17 October 2014
5. Masanobu Yonenaga, Tokyo Metropolitan University, Tokyo, Japan, 9 October–8 November 2014

## STAFF

### Researchers

1. Asst. Prof. Marko Bračko\*
2. Prof. Vladimir Cindro
3. Prof. Andrej Filipič
4. Prof. Boštjan Golob\*
5. Dr. Andrej Gorišek
6. Prof. Borut Paul Kerševan\*
7. Prof. Samo Korpar\*
8. Dr. Gregor Kramberger
9. Prof. Peter Križan\*
10. Asst. Prof. Igor Mandić
11. Prof. Marko Mikuž\*, Head
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13. Asst. Prof. Tomaž Podobnik\*
14. Prof. Marko Starič
15. Prof. Marko Zavrtanik
16. Prof. Danilo Zavrtanik\*
17. Asst. Prof. Anže Zupanc
18. Asst. Prof. Dejan Zontar\*

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19. Dr. Boštjan Maček
20. Dr. Marko Petrič
21. Dr. Andrej Studen

### Postgraduates

22. Jyoti Prakash Biswal, B. Sc.
23. Maksym Deliyergiyev, B. Sc.
24. Luka Kanjir, B. Sc.
25. *Jure Klučar, B. Sc., left 01. 11. 14*
26. Matic Lubej, B. Sc.
27. Manca Mrvar, B. Sc.
28. Miha Muškinja, B. Sc.
29. Tara Nanut, B. Sc.
30. Eva Ribežl, B. Sc.
31. Grygorii Sokhrannyi, B. Sc.
32. *Aleš Svetek, M. Sc., left 01. 03. 14*
33. *Dr. Luka Šantelj, left 01. 07. 14*
34. Tina Šfiligoj, B. Sc.
35. Elvedin Tahirović, B. Sc.

### Technical and administrative staff

36. Andreja Butina
37. Jurij Eržen
38. Erik Margan

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

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- at  $\sqrt{s} = 8$  TeV", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 89, no. 3, pp. 032002-1-032002-23, 2014.
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- AUGER Collaboration, J. R. T. De Mello Neto *et al.*, "Studies of cosmic rays at the highest energies with the Pierre Auger Observatory", In: *2nd International Conference on New Frontiers in Physics, Kolymbari, Crete, Greece, August 28 - September 5, 2013*, [EPJ] Web of conferences, vol. 71), L. Bravina, ed., Les Ulis, EDP Sciences, 2014, vol. 71, pp. 00036-p.1-00036-p.12.
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## MENTORING

1. Marko Petrič, *Measurement of CP violation in weak decays of  $B^0 \rightarrow K^+ \pi^- \pi^0$  with the Belle detector*: doctoral dissertation, Ljubljana, 2014 (mentor Marko Starič).
2. Gašper Kuček Mezek, *Simulation of micro black hole evaporation and interaction in the Earth's atmosphere*: master's thesis, Nova Gorica, 2014 (mentor Danilo Zavrtanik).
3. Matic Lubej, *A study of measurement of the CP symmetry violation in  $D^0 \rightarrow \pi^0 \pi^0$  with the Belle II detector*: master's thesis, Ljubljana, 2014 (mentor Anže Zupanc).
4. Manca Mrvar, *Simulations of E-TCT measurements with heavily irradiated silicon detectors*: master's thesis, Ljubljana, 2014 (mentor Igor Mandić; co-mentor Gregor Kramberger).
5. Miha Muškinja, *Multiplication of Charge Carriers in Diamond Detectors*: master's thesis, Ljubljana, 2014 (mentor Marko Mikuž; co-mentor Gregor Kramberger).
6. Petra Rogan, *Dosimetric evaluation of MOSFET dosimeters and a system for the clinical in vivo dosimetry at a linear accelerator*: master's thesis, Ljubljana, 2014 (mentor Peter Križan; co-mentor Božidar Casar).
7. Sabina Steržaj, *Artifacts comparison on 2D and 3D FLAIR pulse sequence of head MRI at multiple sclerosis*: master's thesis, Ljubljana, 2014 (mentor Dejan Žontar; co-mentor Aleš Koren).
8. Igor Šabič, *Study of the effect of anti-scatter grid use in conventional paediatric radiology*: master's thesis, Ljubljana, 2014 (mentor Dejan Žontar; co-mentor Damjana Ključevšek).



# DEPARTMENT OF INORGANIC CHEMISTRY AND TECHNOLOGY K-1

*The Department of Inorganic Chemistry and Technology is one of the leading groups in the world for 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 30 years. It is also active in the field of education and in the field of the promotion of natural sciences among students at colleges and elementary schools.*



Head:

**Asst. Prof. Gašper Tavčar**

During the investigation of reactions between  $\text{XeF}_2$ ,  $\text{MnF}_3$  and UV-irradiated elemental fluorine in anhydrous hydrogen fluoride as a solvent, single crystals of  $[\text{XeF}_5]_2[\text{MnF}_6]$ ,  $[\text{XeF}_5][\text{MnF}_5]$  and  $[\text{XeF}_5]_4[\text{Mn}_8\text{F}_{36}]$  were prepared and their crystal structures determined. Crystals of  $[\text{XeF}_5]_2[\text{MnF}_6]$  consist of  $[\text{MnF}_6]^{2-}$  anions and  $[\text{XeF}_5]^+$  cations. The main structural feature of  $[\text{XeF}_5][\text{MnF}_5]$  are infinite  $[\text{MnF}_5]_n^{n-}$  chains of distorted  $[\text{MnF}_6]$  octahedra joined via cis vertexes, while  $[\text{XeF}_5]^+$  cations compensate the negative charge of each octahedron. The crystal structure of  $[\text{XeF}_5]_4[\text{Mn}_8\text{F}_{36}]$  consists of previously unknown, discrete octameric  $[\text{Mn}_8\text{F}_{36}]^{4-}$  anions. Each of them is constructed from eight  $\text{MnF}_6$  octahedra.

Besides the previously known  $[\text{Ti}_8\text{F}_{36}]^{4-}$  anion, the herein reported  $[\text{Mn}_8\text{F}_{36}]^{4-}$  anion represents the largest known example of discrete oligomeric species found in fluoride compounds with the metal in the oxidation state four.

Igor Shlyapnikov, Evgeny Goreshnik, Zoran Mazej, members of the Department of Inorganic Chemistry and Technology, received the award of the Slovenian Research Agency (ARRS) for an exceptional scientific achievement in 2013 in the field of chemistry (Structural architecture of ternary titanium(IV) fluorides) in the scope of "Excellence in Science 2013". For their achievements in the research of reactions of compounds with titanium(IV) fluoride in anhydrous media, the postgraduate student Igor Shlyapnikov (under the supervision of Dr. Zoran Mazej) received an acknowledgement of the Jožef Stefan International Postgraduate School for exceptional achievements in 2014.

**Igor Shlyapnikov, Evgeny Goreshnik and Zoran Mazej received the award of the Slovenian Research Agency (ARRS) for an exceptional scientific achievement in 2013 in the field of chemistry**

We carried on our research work by exploring the thermal reactions between a medium-strong Lewis base xenon difluoride ( $\text{XeF}_2$ ) and titanium tetrafluoride ( $\text{TiF}_4$ ). Using Raman spectroscopy, we focused our investigations on clarifying the complex reaction mechanisms that lie behind the formation of a new type of Xe(II) salts with polymeric anions:  $[\text{XeF}_2]_2[\text{Ti}_9\text{F}_{38}]$  and  $[\text{Xe}_2\text{F}_3][\text{Ti}_8\text{F}_{33}]$ . The 1-D and 2-D polyanions found in the structures of these compounds show an unexpected ability to maintain relatively high ionization forms of  $\text{XeF}_2$ . To date, this process was accomplished only by using the strongest known Lewis acids (e.g.,  $\text{SbF}_5$ ). The synthetic and crystallization methods developed open up new possibilities in terms of making more thermodynamically stable  $[\text{XeF}]^+$  and  $[\text{Xe}_2\text{F}_3]^+$  salts, containing other anions of weaker Lewis acids.

The syntheses of the compounds with  $\text{XeF}_2$  as a ligand belong to the research field of the noble gases. We prepared a compound with the composition  $[\text{Bi}(\text{XeF}_2)_3][(\text{BiF}_6)]_3$ . It is particularly interesting because of the central metal. The coordination sphere of the  $\text{Bi}^{3+}$  consists of three fluorine atoms from  $\text{XeF}_2$  molecules and six fluorine atoms from  $\text{BiF}_6^-$  anions. In this way we can open up a new area of research with the main group metals with oxidation state three, which are suitable for the coordination of  $\text{XeF}_2$ . Main structural features of the compounds  $[\text{Hg}(\text{XeF}_2)_5][(\text{AF}_6)]_2$  ( $A = \text{P}, \text{As}, \text{Sb}$ ) are the formation of the chains of mercury atoms connected *via*  $\text{XeF}_2$  molecules.

We have continued the research of hybrid materials formed by the reactions between metal halogenides and N-heterocyclic carbenes and successfully prepared some new compounds with antimony(III) fluoride. The solubility in non-polar solvents was drastically increased by the use of the TMEDA ligand that was coordinated to antimony(III) fluoride. As a consequence reactions in non-polar solvents led to an unusual coordination. The

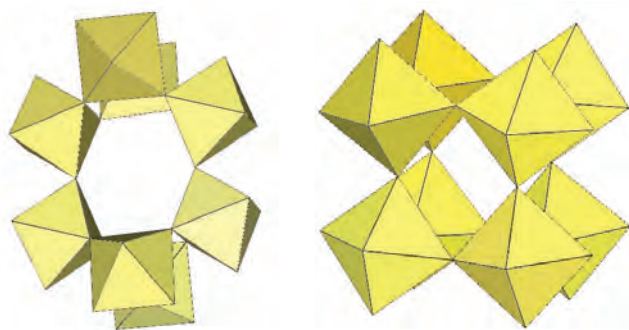


Figure 1: Oligomeric  $[\text{Mn}_8\text{F}_{36}]^{4-}$  anion (a) determined in the crystal structure of  $[\text{XeF}_5]_4[\text{Mn}_8\text{F}_{36}]$  and already known  $[\text{Ti}_8\text{F}_{36}]^{4-}$  anion (b) determined in the crystal structures of  $\text{K}_4\text{Ti}_8\text{F}_{36} \cdot 8\text{HF}$  and  $\text{Rb}_4\text{Ti}_8\text{F}_{36} \cdot 6\text{HF}$  (I. Shlyapnikov, E. Goreshnik, Z. Mazej, *Chem. Commun.* 2013, 49, 2703-2705).



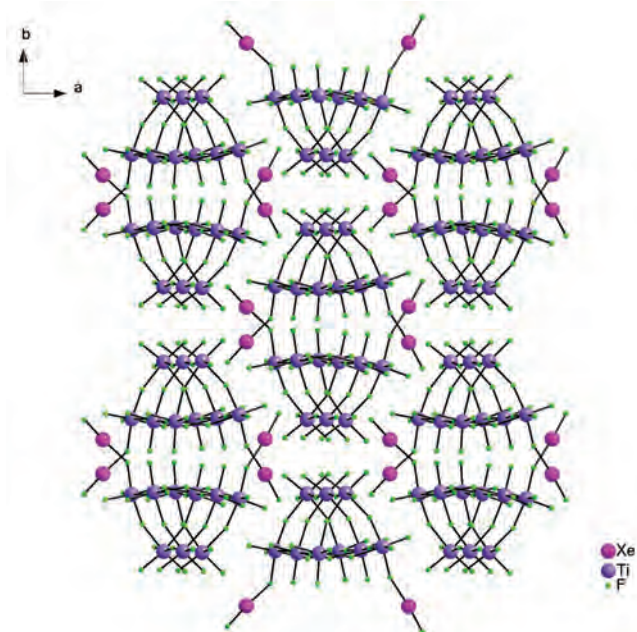


Figure 2: Columnar structure found in  $[XeF]_2[Ti_3F_{38}]$ ; view along the  $c$ -axis

most interesting is the compound that was formed due to rearrangement on the imidazole ring and its abnormal coordination to the metal center.

The structural investigations of copper(I) pi-complexes with N-allylthiadiazole and tetrazoles have been continued. The most interesting result is the formation of the  $Cu_2SiF_6 \cdot 2L \cdot 2H_2O \cdot C_2H_5NO$  ( $L = N$ -allylthiadiazole) compound. Acetamide ( $C_2H_5NO$ ) appeared in the reaction mixture as a consequence of the slow hydrolysis of an acetonitrile solvent. The water molecules, acetamide moiety, NH-groups of the ligand and the  $SiF_6^{2-}$  anions form an unprecedented system of hydrogen bonds.

Detailed spectroscopic investigations of nanostructured fluoride aerogels based on  $AlF_3$  enabled the identification and differentiation of species formed inside processes that accompany the supercritical drying of fluoride precursors in anhydrous alcoholic media. The two main side processes are hydration and hydroxylation, the latter resulting from the partial hydrolysis of the fluoride phase. In alcoholic media containing methanol, the partial exchange of surface OH groups with methoxide (OMe) groups also takes place. In comparison with the  $H_2O$  and OH groups located in the interior of the basic nanoparticles, surface  $H_2O$ , OH and OMe species exhibit a lower stability and can be removed by a thermal or chemical treatment under relatively mild conditions. The internal  $H_2O$  and OH species are primarily located within the hexagonal channels characteristic for the  $\beta$ - $AlF_3$  structure. The effective removal of these species requires more severe conditions, which usually leads to the loss of the basic nanostructure. A better understanding of these

processes will help in the preparation of fluorides with an activated surface and a conserved initial nanostructure.

The novel composite  $MoS_2(IF)/C$  material and the urchin-like  $MoS_2$  were synthesised and characterised.  $MoS_2(IF)/C$  is the first single-synthesis-step composite containing  $MoS_2$  inorganic fullerenes (IF) interconnected with carbon. Inorganic fullerene units of approximately 12 nm in diameter are interconnected by amorphous carbon inclusions and form agglomerates that are 50–100  $\mu m$  in size. The urchin-like  $MoS_2$  catalyst exhibited a higher activity compared to the commercial  $MoS_2$  powder in the hydrodeoxygenation of liquefied wood. The oxygen content decreased from 43.3 % to 8.2 % (wt.), while the residual phenolic oxygen is not removable with this particular catalyst. The observed catalytic performance may provide new solutions in terms of biofuel processing. This research work was done in cooperation with the National Institute of Chemistry, Slovenia.

The cooperation with the National Academy of Sciences of the Ukraine continued with activated carbons with a specific surface area in the range from 980 to 2100  $m^2/g$ , which were produced from cornelian cherry stone, the fruit-processing waste, by thermal processing. The chemical activation was performed at a different mass ratio of raw material to phosphoric acid, which resulted in a different activated carbon total pore volumes in the range from 0.44 to 0.77  $cm^3/g$ . The adsorption capacity of the produced carbons for ions of the heavy metals  $Cd^{2+}$ ,  $Cr^{3+}$ ,  $Ni^{2+}$ ,  $Cu^{2+}$  and  $Zn^{2+}$  in water solutions were determined. The distinctive character of the adsorption of  $Cd^{2+}$  compared to the adsorption of other ions offers the possibility of using carbons from cornelian cherry stone to separate the cadmium ions from other heavy-metal ions.

A principle of redox back titration used for the determination of ethanol or phenol contents with the emphasis on the stoichiometry of chemical reactions was described. The (in)stability of aqueous suspensions of nanoparticles was investigated in collaboration with the Materials Synthesis Department (K8).

Within the project J1-4288 "Speciation and interactions of chemical contaminants at trace level in aqueous media to support the development of cost-effective removal technologies" the work was performed in cooperation with the Department for Environmental Sciences (O2). A series of experimental tests was performed on a laboratory and semi-industrial scale researching the influence of specific pollutants on Hg-removal efficiency from the model gas which simulated the flue gas from thermal power plants.

In the topic of process safety we continued with the EU 7FP project TOSCA (Total Operations Management for Safety Critical Activities) in which we participate as a partner. The project deals with the integration of the individual management aspects of industrial operations as a total safety, quality and productivity management system (at the company level), covering the whole life cycle of the product. We provided inputs mainly at specifying the "T" (for TOSCA) concept of the safety management, specifically for the level of process equipment management (enumerating, procedures, maintenance, inspections, hazards, visualization) and leading the planning for 11 demonstration case studies of TOSCA products, where we lead the coordination among industrial partners' needs with the expected functionality of the developed products, or integrated solutions.

We continued work within the EU COST action ES 1006 - Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments. Within the action we participate in the assessment of the accuracy of the existing hazardous substances atmospheric dispersion models into the ambient air in a complex/urban environment, as well as in the preparation of the best-practice guidelines for modelling. In that scope we participate during the preparation of the related guidelines within the chapter on risk assessment, specifically hazard identification, and hazardous-substances release conditions with relevance for the modelling of their dispersion into the air.

In this year we were in the end-user platform of the EU 7FP project EDEN (End User Driven Demo for CBRNe), which started in September 2013. In the project, which deals with the assessment and preparedness for terrorist risks (aspect of security), we participate on the basis of our previous experiences in the assessment of such threats to industrial operations.

For the Slovenian Environment Agency (ARSO) we took part in the project of the reviewing of the Safety Case reports for the lower-tier establishments (according to the Seveso directive) as part of the licensing procedures.

The IPA project Adriacold "Diffusion of cooling and refreshing technologies using the solar energy resource in the Adriatic regions", started in October 2012, was continued in 2014 with partners from Italy, Slovenia, Croatia, Bosnia & Herzegovina and Albania. The JSI leads the Work Task "Monitoring and data mining", which comprises the planning and systematic collection of performance data for six pilot and testing solar cooling plants (in the cities of Dubrovnik and Rijeka (Croatia), Piran (Slovenia), Bazovica, Rimini and Bari (Italy)), and data analysis with the addition of the automatic display of key operational performance indicators in a web application. From May to September 2014 the project partners managed to install and put into operation half of the planned pilot plants (locations Dubrovnik, Rijeka and Piran), so the first useful data started to pour in for checking their consistence and data processing. The data shows important differences between the installations due to the different end-uses of the produced cold (a computing centre, a spa, and a kindergarten).

As part of the cooperation in the 30-months international project EMILIE (Enhancing Mediterranean Initiatives Leading Innovation and SMEs to Building Energy Efficiency Technologies, [www.emilieproject.eu](http://www.emilieproject.eu)) there was a pilot facility Infrason built in the first half of 2014. It was designed as a research and educational energy polygon based on the integration of the most advanced solar thermal technologies into a unified system of heating and cooling using solar energy, thus showing an example of the use 'of the sun as infrastructure'. The system was put into operation in July 2014, since then continuous measurements have been carried out as part of a detailed analysis of the process and energy indicators as well as the optimization of the system. There are heating and cooling systems, incorporating the latest solar technologies and systems for the use of waste heat, tested in the pilot facility as well as the facility that is used for education purposes, primarily targeted at small and medium-sized enterprises and administrative bodies that are responsible for the promotion of energy efficiency and the use of renewable energy sources. One of the outcomes of the successful implementation of the pilot facility is established cooperation in the testing and development of new designs of solar thermal technologies.

The work within the project "Methodology of fixation of CO<sub>2</sub> on fly ash" was continued and finished along with the partners from the Razvojni center Energija d.o.o. (RCE) (Development Centre Energy d.o.o.), where the department researchers provided consulting and support work for technology development on the pilot, semi-industrial and industrial scale based on laboratory-test findings. Based on the measurements on the semi-industrial plant a mobile industrial-scale plant for absorption solution preparation using fly ash, CO<sub>2</sub> absorption using this solution, and the separation of the product (carbonate) from the absorption slurry, was designed.

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 men-



Figure 3: A view to the solar thermal collectors filed ('roll-bond' type) at the JSI headquarters in Ljubljana (photo: M. Smerke)

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### Successful implementation of the pilot facility EMILIE Infrason as a platform for the evaluation of innovative technologies in the field of energy-efficient buildings

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Figure 4: Installation with the adsorption chillers and heat storage (photo: M. Smerke)

tors 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. With the demonstrations of chemical experiments we participated at the 20th Slovenian Science Festival, organized by the Slovenian Science Foundation and at the Researchers Night in Ljubljana and other events. Some of the activities of the School of Experimental Chemistry were carried out within the project, which is funded by the JSI and the City of Ljubljana.

### Some outstanding publications in the past years

1. Radan, K., Goresnik, E., Žemva, B.: Xenon(II) Polyfluoridotitanates(IV): synthesis and structural Characterization of  $[\text{Xe}_2\text{F}_3]^+$  and  $[\text{XeF}]^+$  Salts, *Angew. Chem.* 53 (2014) 13715-13719
2. Veryasov, G., Grilc, M., Likozar, B., Jesih, A.: Hydrodeoxygenation of liquefied biomass on urchin-like  $\text{MoS}_2$ . *Catalysis Comm.*, 46 (2014), 183-186
3. Ponikvar-Svet M., Zeiger D. D., Keating L. R., Liebman J. F., Interplay of thermochemistry and structural chemistry, the journal (volume 24, 2013, issues 3-4) and the discipline, *Structural chemistry*, 25 (2014), 1581-1592
4. Shlyapnikov, I., Goresnik, E. A., Mazej, Z.: The cubic  $[\text{Ti}_8\text{F}_{36}]^{4-}$  anion found in the crystal structures of  $\text{K}_4\text{Ti}_8\text{F}_{36}\cdot 8\text{HF}$  and  $\text{Rb}_4\text{Ti}_8\text{F}_{36}\cdot 6\text{HF}$ , *Chem. Comm.*, 49 (2013), 2703-2705
5. Tavčar, G., Žemva, B.:  $[\text{Li}(\text{XeF}_2)_n](\text{AF}_6)$  (A = P, As, Ru, Ir), the first xenon(II) compounds of lithium, Synthesis, Raman spectrum and crystal structure of  $[\text{Li}(\text{XeF}_2)_3](\text{AsF}_6)$ , *Inorg. Chem.*, 52 (2013), 4319-4323

### Awards and appointments

1. Igor Shlyapnikov, Evgeny Goresnik and Zoran Mazej received recognition from Research Agency of the Republic of Slovenia for outstanding achievement in 2013 in the field of chemistry (Structural architecture of ternary titanium (IV) fluorides) as part of "Excellent in Science 2013".
2. Igor Shlyapnikov, a postgraduate student under the supervision of dr. Zoran Mazej, received the award of the International Postraduate School Jožef Stefan for exceptional achievements in the year 2014.

### Organization of conferences, congresses and meetings

1. EMILIE (MED programme): Jožef Stefan Institute 3rd Meeting of Steering Committee and 3rd Capitalization meeting, Ljubljana, Slovenia, 10-11 June 2014

## INTERNATIONAL PROJECTS

1. Export of the Fluorinated Carbons  
Dr. Zoran Mazej  
Foreign buyers
2. 7FP - TOSCA; Total Operations Management for Safety Critical Activities  
Asst. Prof. Marko Gerbec  
European Commission
3. 7FP - FluoCoorChem; Fluorinated Weakly Coordinating Anions for Coordination Chemistry of Unusual Ligands  
Prof. Boris Žemva  
European Commission
4. COST ES1006; Evaluation, Improvement and Guidance for the Use of Local-scale Emergency Prediction and Response Tools for Airborne Hazards in Built Environments  
Asst. Prof. Marko Gerbec  
COST Office
5. IPA ADRIATIC; ADRIACOLD - Diffusion of Cooling and Refreezing Technologies using the Solar Energy resources in the Adriatic Regions  
Asst. Prof. Gašper Tavčar  
Ministry of Economic Development and Technology
6. MED - EMILIE; Enhancing Mediterranean Initiatives Leading SMEs to Innovation in Building Energy Efficiency Technologies  
Asst. Prof. Gašper Tavčar  
STC Programme MED
7. Preparation of Agro-based Active Carbons by Phosphoric Acid Activation and their Application for Heavy Metal Removal and Improvement of Transition Metal Catalysts  
Dr. Adolf Jesih  
Slovenian Research Agency

## RESEARCH PROGRAM

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

## R & D GRANTS AND CONTRACTS

1. Speciation and Interactions of Chemical Contaminants at Trace Level in Aqueous Media to Support the Development of Cost-effective Removal Technologies  
Dr. Andrej Stergaršek

## NEW CONTRACTS

1. Fly ash  $\text{CO}_2$  fixation methodology  
Dr. Robert Kocjančič  
RCE - Research Centre Energy Ltd
2. Participation within the Project School of Experimental Chemistry, Financed by City of Ljubljana, Activities in the field of Technics and Experimentation for Pupils in 2014  
Asst. Prof. Gašper Tavčar  
Slovensko društvo ljubiteljev kemije
3. Preparation of the Risk Reduction Plan for the Environment for the Planned Technical Gases production plant at land parcel 4d, industrial zone Štore II.  
Asst. Prof. Marko Gerbec  
Istrabenz plini, d. o. o.
4. Update of the Threat Assessment for Natural Gas Distribution Pipeline Network and Preparation of the Threat Assessment for Planned Pipeline Network Expansion  
Asst. Prof. Marko Gerbec  
Plinovodi, d. o. o.



## VISITORS FROM ABROAD

1. Dr. Piotr Leszczynski and Tomasz Gilewski, University of Warsaw, Warsaw, Poland, 23 March–14 April 2014
2. Andrzej Mika, Michal Masny, Wojciech Adamczyk and Sandra Lepak, University of Warsaw, Warsaw, Poland, 1–10 July 2014
3. Prof. Wojciech Grochala, University of Warsaw, Warsaw, Poland, 2–11 July 2014
4. Anja Starec, Fabio Tomasi, AREA, Trieste, Italy, 27 October 2014
5. Amirthapandian Karthikeyan, TU Dresden, Germany, 1 September–31 October 2014
6. Marc Vigneron, Pierre Charles, Yannick Goetz, Viessmann, France, 21 November 2014
7. Prof. dr. Herbert W. Roesky, University of Göttingen, Göttingen, Germany, 2 December 2014

## STAFF

### Researchers

1. Asst. Prof. Marko Gerbec
2. Asst. Prof. Evgeny Goreshnik
3. Dr. Adolf Jesih
4. Dr. Robert Kocjančič
5. Dr. Zoran Mazej
6. Asst. Prof. Maja Ponikvar-Svet
7. Asst. Prof. Tomaž Skapin
8. Asst. Prof. Gašper Tavčar, Head
9. Dr. Melita Tramšek

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10. Blaž Alič, B. Sc.
11. Alenka Koblar, B. Sc.
12. Dr. Matic Lozinšek

13. Kristian Radan, B. Sc.
14. Igor Shlyapnikov
15. *Gleb Veryasov, left 01. 08. 14*
16. Žiga Zupanek, B. Sc.

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20. Peter Frkal, B. Sc.
21. Pero Kolobaric
22. Robert Moravec
23. Mira Zupančič

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

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2. Erik Stritih, *Assessment of the possibility to reduce fuel consumption in personal vehicles using dedicated additives and devices*: master's thesis, Ljubljana, 2014 (mentor Marko Gerbec; co-mentor Robert Kocjančič).

3. Sašo Marn, *Life cycle assessment of a Minidil rectifier bridge*: master's thesis, Ljubljana, 2014 (mentor Marko Gerbec; co-mentors Robert Kocjančič, Damjan Bizjak).

# DEPARTMENT OF PHYSICAL AND ORGANIC CHEMISTRY

# K-3

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

Experimental research in the field of physical chemistry is oriented to various types of corrosion protection for materials, as well as of mechanisms of degradation for materials in various environments.

Biomedical materials must fulfil strict requirements of high corrosion and wear resistance. Three main groups of materials are used for joint prostheses, including alloys based on titanium, cobalt and stainless steel. In a long-term collaboration with the Valdoltra Orthopaedic Hospital, studies devoted to the effects of physiological conditions on the corrosion stability of the main orthopaedic alloys are carried out. In addition to studies of commercial alloys, studies oriented to the development of new materials for biomedical applications are also being performed. Within the project financed by the European Research Area (ERA) we have investigated a novel alloy for biomedical applications, Ti-20Nb-10Zr-5Ta. This alloy exhibits better mechanical properties, i.e., a lower elastic modulus and a higher hardness, than commercial titanium alloys. At the same time there is more corrosion protection under simulated physiological conditions.

During the in-vivo functioning of total joint prostheses the combination of corrosion and wear processes often occurs. As these processes determine the long-term stability and survivorship of prostheses it is important to evaluate them and to assess the related changes to the prosthetic components and the periprosthetic biological environment. Using a coordinate measuring machine we have developed a method for measuring the volumetric and linear wear of the femoral head of total hip prostheses. The measured data are then used to derive the in-vivo wear rate of a particular material. As wear rate affects the survivorship, the data are important to assess the long-term performance of prostheses and to compare the wear rates of different types of prostheses

Another group of materials that is the focus of our investigations includes materials important for use in industry, mainly alloys based on aluminium, copper and zinc. Due to their beneficial properties aluminium and its alloys are used in numerous applications in civil engineering, the automotive and aerospace industries, and the food and electronic industries. These materials exhibit low density, high tensile strength, excellent thermal and electrical conductivity and a high strength-to-weight ratio. Desirable mechanical properties are achieved by alloying with copper, manganese, magnesium or zinc. On the other hand, alloying can worsen the corrosion resistance of aluminium as intermetallic sites represent the initial sites for corrosion. For many decades chromate coatings represented the most effective corrosion protection for aluminium alloys. In the European Union their use is banned or restricted due to their toxicity. Today, new alternatives for conversion chromate coatings are being investigated, which would achieve a comparable corrosion protection, while being environmentally acceptable. In that context the development of sol-gel coatings is important. In our laboratory we are devoted to the development of hybrid sol-gel coatings that enable the effective corrosion protection of aluminium and its alloys. A two-step procedure for synthesizing a new type of hybrid coating was developed. The coatings were synthesized from tetraethyl orthosilicate (TEOS), 3-(trimethoxysilyl)propyl methacrylate (MAPTMS) and zirconium(IV) propoxide (ZTP). Zirconium(IV) propoxide was chelated with methacrylic acid. The synthesis, which proceeded at room temperature, was optimized using *in situ* Fourier transform infrared spectroscopy (FTIR). The effects of MAPTMS/TEOS ratios, the addition of water, the ageing time and the curing parameters were investigated. Each step of the synthesis was additionally investigated using proton nuclear magnetic resonance spectroscopy in order to follow the changes in chemical bonding and structure. Once deposited in the form of a coating on aluminium alloys, these TMZ coatings offer high



Head:  
**Prof. Ingrid Milošev**

**Hybrid sol-gel coatings based on silicon and zirconium offer excellent corrosion protection for aluminium alloys in chloride solutions. The synthesis procedure is protected under an international patent application.**

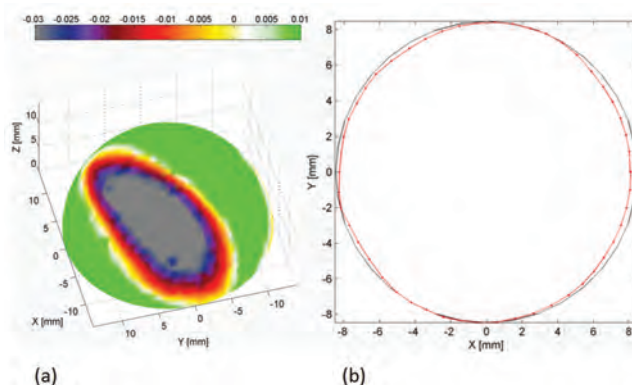


Figure 1: Example of measurement of (a) three-dimensional volumetric and (b) linear wear of retrieved femoral head of total hip prosthesis using a coordinate measuring machine.

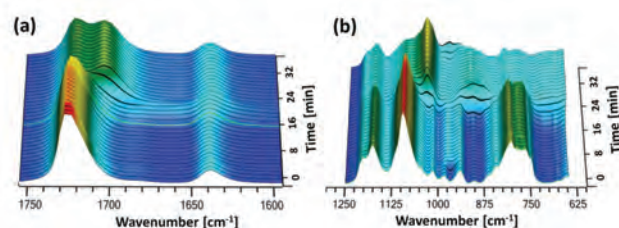


Figure 2: In-situ Fourier transform infrared analysis during synthesis of hybrid TMZ sol-gel coating presents time dependence of compositional changes upon the addition of acid catalyst to the mixture of tetraethyl orthosilicate (TEOS) and 3-(trimethoxysilyl)propyl methacrylate (MAPTMS) at 60 °C.

**Benzotriazole (as an excellent corrosion inhibitor) and chloride (as a corrosion activator) are bonded more strongly at defect sites than at regular sites at the copper surface; however, the bonding enhancement is stronger for benzotriazole, which indicates its ability to passivate the surface.**

minute of immersion in the inhibitor solution. Studies will be complemented with a combination of carboxylic acids and traditional organic inhibitors (i.e., molecules that have the ability to inhibit the corrosion), which is expected to achieve more effective and longer-lasting protection.

We continued with a theoretical study of organic corrosion inhibitors at the molecular level, aiming to discern the fundamental principles that govern their corrosion-inhibition characteristics. In the past few years we have studied by means of first-principle density-functional-theory (DFT) based computer modelling the interaction of several azole-type corrosion inhibitors with surfaces of copper, iron, and aluminium. Our findings indicate that the inhibitor-surface bonding strongly depends on the type of metal. In the preceding year we addressed the role of surface defects on copper surfaces and compared the differences between the adsorbate-surface bonding of benzotriazole and chloride; the former is an outstanding corrosion inhibitor and the latter is a common corrosion activator. The issue is of importance, because under-coordinated surface defects are usually far more reactive than perfect facets; hence they are also plausible microscopic sites for potential corrosion attack. We found that the bonding enhancement near defects is stronger for benzotriazole than for chloride, which indicates the ability of benzotriazole to passivate reactive surface sites. We also showed that under-coordinated surface defects promote the dissociative adsorption of benzotriazole (N–H bond cleavage), whose importance stems from the fact that only in this form can benzotriazole make bonds that are strong enough to rival the Cl–Cu surface interaction.

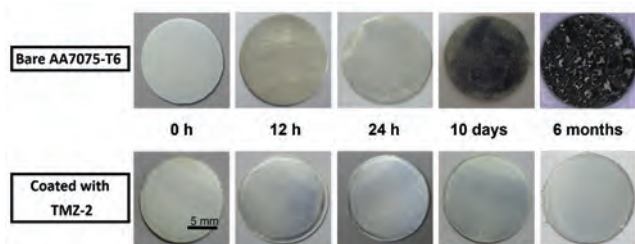


Figure 3: Images of samples immersed in solution simulating aircraft conditions for different periods of time: bare aluminium alloy 7075-T6 and coated with hybrid TMZ-2 coating prepared from organically modified siloxane precursors and zirconium(IV) propoxide.

**We have predicted that the presence of HOSO-water and CH<sub>3</sub>SO-water complexes can be identified by infrared spectroscopic detection under laboratory conditions as well as in atmospheric observations.**

corrosion protection, as shown by the studies in solution simulating aircraft conditions. The results of electrochemical studies were also confirmed by long-term, salt-spray-chamber and immersion testing. This innovation was included in the programme Bastille LCC and the international patent application was filed in 2014. Another alternative to chromate coatings are conversion coatings based on rare-earth nitrate and chloride salts. The inhibition effectiveness of the coatings is dependent on the bath conditions, i.e., the immersion time and the temperature. Special attention was devoted to the preparation of mixtures of different salts of cerium and lanthanum.

Copper is an excellent electrical and thermal conductor and so it is often used for the production of wires and pipes. Alloying with Zn, Sn, and Ni improves the mechanical properties of the metal, while it retains its excellent corrosion resistance under more severe service conditions. Alloys of copper are often used for structures open to the atmosphere, for example, in architecture and for sculptures. We have studied methodologies for their protection by increasing the hydrophobicity of the surface, thus not wetted by aqueous liquids and less prone to degradation in urban environments. This was achieved by the self-assembling of a layer of carboxylic acids at the metal surface. The effectiveness of the protection was tested in simulated urban rain. It increases with the length of the aliphatic tail of the carboxylic acid. All acids form layers with a contact angle greater than 90°. The process of self-assembling is fast, as corrosion protection was achieved after only one

minute of immersion in the inhibitor solution. Studies will be complemented with a combination of carboxylic acids and traditional organic inhibitors (i.e., molecules that have the ability to inhibit the corrosion), which is expected to achieve more effective and longer-lasting protection.

Theoretical investigations are very important for understanding the mechanism of physico-chemical reactions in atmospheric chemistry. Atmospheric nucleation processes are not yet well understood and are difficult to probe by experimental means. High-level density functional and ab-initio calculations were utilized as a powerful tool for gaining insights about the nucleation mechanism to accurately describe the very first step of particle formation, i.e., the clustering of the first few atmospheric species from the gas phase. We presented a comprehensive series of electronic structure calculations on small clusters, in particular, the H-bonded complexes of HOSO and CH<sub>3</sub>SO radicals with one and two molecules of H<sub>2</sub>O. A general characteristic feature of the minimum energy structure complexes is the cyclic double hydrogen bonding for 1:1 complexes and cyclic triple hydrogen bonding for 1:2 complexes. The stabilization of some complexes relative to others due to their hydration significantly affects the overall processes of new particle formation in the atmosphere and changes the photochemical features related to the free radicals. The infrared (IR) spectral shifts and intensities for the water complexes in comparison with respect to the corresponding monomers are substantially pronounced for the OH stretching vibrations. The present data suggest that IR spectroscopy can be powerful tool in the



IR spectroscopic detection of the HOSO-water and  $\text{CH}_3\text{SO}$ -water complexes under laboratory conditions as well as in atmospheric observations. On the other hand, vertical electronic excitation energies indicate an insignificant spectral shift in comparison to the free radicals, which consequently suggests that the radicals and complexes are experimentally indistinguishable using standard UV/Vis absorption spectroscopy.

In the framework of the Laboratory for Organic and Bioorganic Chemistry we continued the investigation on applying the principles of green chemistry to the transformations of organic compounds.

We developed the method for aerobic oxidative iodination of organic compounds using air oxygen as the terminal oxidant catalysed by ammonium nitrate under acidic conditions. The reaction system: *air* / *ammonium nitrate (cat)* / *molecular iodine* /  $\text{H}_2\text{SO}_4$  (*cat*) was used for selective and efficient iodination of activated aromatics and various ketones to alpha iodo substituted derivatives. A new method for the selective chlorination of aryl methyl ketones using the reaction system *air* / *ammonium nitrate (cat)* / *molecular iodine (cat)* / 36% aqueous HCl was verified on comprehensive type of ketones, including those bearing heteroatoms, such as nitrogen or sulphur, thus selectively and efficiently preparing chloromethyl derivatives. The reaction course was found to be the aerobic oxidative iodination of alpha to carbonyl position followed by a halogen-exchange process and oxidative regeneration of released iodide, so continuing the process. The method opens up numerous possibilities for the aerobic oxidative functionalization of the alpha-to-carbonyl position in ketones with other functional groups.

The discovery that N-halo organic compounds could be efficient catalysts for various transformations of alcohols, thus forming new C-C or C-heteroatoms bonds in target molecules, was verified on a comprehensive type of benzyl alcohols reacting with alkenes, 1,3-diketones, amines, alkyl alcohols or trimethylsilanes as electron-rich molecules. The reactions were efficiently performed in solvent-free reaction conditions. We developed a new method for the synthesis of organic peroxides bearing potential bioactivity using in situ concentrated hydrogen peroxide thus improving considerably the selectivity of the dihydroperoxide formation.

On the basis of a discovered innovation the spin-out company RGA was opened, which will be operating on agro chemistry and biotechnology. In the framework of the Centre of Excellence CIPKeBiP and the collaboration of the high-tech company ACIS BIO we were continuing investigations of the directed synthesis building blocks of potential bioactive compounds from the family of pantothenic acid and derivatives of maleic acid as precursors in polyketide biosynthesis. We were developing new products used in non-human cosmetics for the company ECOT.

Co-workers of the department are engaged at the Jožef Stefan International Postgraduate School and at the Faculty of Chemistry and Chemical Technology at the University of Maribor.

## Some outstanding publications in the past year

- Rodič, P., Iskra, J., Milošev, I.: Hybrid organic-inorganic sol-gel coatings for protection of AA7075-T6 alloy against corrosion in Harrison's solution, *J. Sol-Gel Sci. Technol.*, 70 (2014), 90-103
- Topolovec, M., Cör, A., Milošev, I.: Metal-on-metal vs. metal-on-polyethylene in total hip arthroplasty: Tribological evaluation of retrieved components and periprosthetic tissue, *J. Mech. Beh. Biomed. Mater.*, 34 (2014), 243-252
- Žerjav, G., Milošev, I.: Carboxylic acids as corrosion inhibitors for Cu, Zn and brasses in simulated urban rain, *International Journal of Electrochemical Science*, 9 (2014), 2696-2715
- Peljhan, S., Koller, J., Kokalj, A.: The effect of surface geometry of copper on adsorption of benzotriazole and Cl, *J. Phys. Chem. C*, 118 (2014), 933-943
- Lesar, A., Tušar, S.: Structure, stability and spectroscopic properties of H-bonded complexes of HOSO and  $\text{CH}_3\text{SO}$  with  $\text{H}_2\text{O}$ , *J. Phys. Chem. A*, 118 (2014), 7855-7862

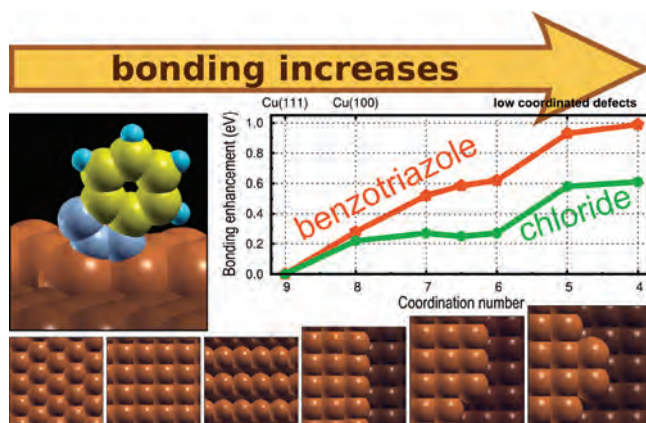


Figure 4: Benzotriazole (outstanding corrosion inhibitor) and chloride (aggressive corrosion activator) bonds stronger to under-coordinated surface defects than to perfect facets on copper surfaces, but the bonding enhancement is stronger for benzotriazole.

**We discovered that some N-halo organic compounds are efficient catalysts for comprehensive transformations of alcohols under solvent-free reaction conditions.**

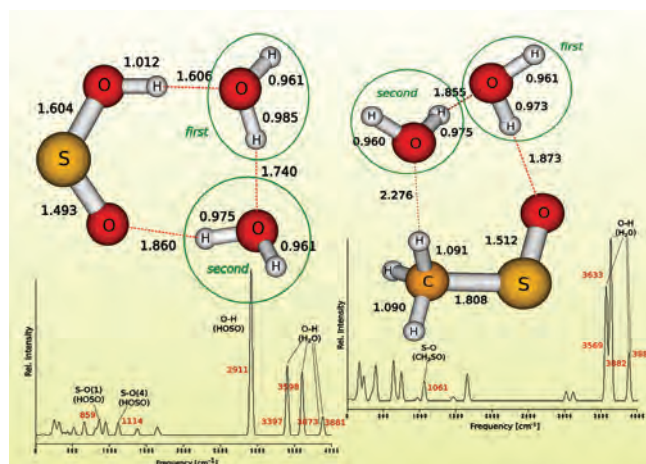


Figure 5: Structures and infrared spectra for the stable 1:2 complexes of HOSO-water and  $\text{CH}_3\text{SO}$ -water



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### Awards and appointments

- Rok Prebil: Pregl Award for Outstanding Doctoral Thesis in Chemistry and Related Sciences, Ljubljana, Slovenia, 2014

## INTERNATIONAL PROJECTS

- CARISMA; Catalytic Routines for Small Molecule Activation  
Asst. Prof. Jernej Iskra  
COST Office
- EUSpec, COST MP1306; Modern Tools for Spectroscopy on Advanced Materials: A European Modelling Platform  
Asst. Prof. Anton Kokalj  
COST Office
- Improvement of Functionality of Biomedical and Engineering Materials  
Prof. Ingrid Milošev  
Slovenian research Agency

## RESEARCH PROGRAMS

- Bioinorganic and Bioorganic Chemistry  
Prof. Stojan Stavber
- Multiphase Nanoarchitectures: Development, Physical-Chemical Characterization and Simulation of Processes  
Prof. Ingrid Milošev

## R & D GRANTS AND CONTRACTS

- Modifications of Surface of Metallic Biomaterials and their Interaction with Bio-environment  
Prof. Ingrid Milošev
- Lightweight Alloys based on Aluminium as Materials with Increasing Potential in Transport Industry  
Prof. Ingrid Milošev
- Development of Molecularly Imprinted Polymers and their Application in Environmental and Bio-analysis  
Asst. Prof. Jernej Iskra
- New Technology for Design of Novel Polyketide Drug-leads with Chemically Amenable Moieties  
Prof. Stojan Stavber

## NEW CONTRACT

- Development of New Synthetic Protocols  
Prof. Stojan Stavber  
ACIES BIO, d. o. o.

## VISITORS FROM ABROAD

- Prof. Shaun Murphree, Fulbright fellowship, Allegheny College, Meadville, PA, USA, 3 February–8 July 2014
- Nicoleta Cotelan, Ph.D. Student, University Babes-Bolyai, Cluj-Napoca, Romania, 2 April–30 June 2014
- Dr. Dominique Cahard, CNRS, COBRA, University of Rouen, Mont-Saint-Aignan, France, 6 June 2014
- Daniela Covaciu Romonti, Postdoctoral Fellowship, University Politehnica of Bucharest, Romania, 17 September 2014–17 January 2015
- Dr. Andrea Gomez Sanchez, INTEMA, Division of Electrochemistry and Corrosion, National University Mar del Plata, Argentina, 20–31 October 2014
- Prof. Philippe Marcus, CNRS, Paris, France, 24 October 2014

## STAFF

### Researchers

- Asst. Prof. Jernej Iskra
- Asst. Prof. Anton Kokalj
- Dr. Antonija Lesar
- Prof. Ingrid Milošev, Head**
- Prof. Stojan Stavber

### Postgraduates

- Jerca Pahor, B. Sc.
- Dunja Peca, B. Sc.
- Matic Poberžnik, B. Sc.

### 9. Dr. Rok Prebil, left 01. 07. 14

- Dr. Peter Rodič
- Katarina Starkl, B. Sc.
- Urša Tiringner, B. Sc.
- Simona Tušar, B. Sc.
- Barbara Volarič, B. Sc.
- Gregor Žerjav, B. Sc.

### Technical officers

- Barbara Kapun, B. Sc.

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## ORIGINAL ARTICLE

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  - Rok Prebil, "Kvaliteta zraka in problematika izpustov trdnih delcev v ozračje", V: *Sodobni pristopi poučevanja prihajajočih generacij*, Mojca Orel, ed., Polhov Gradec, Eduvision, 2014, pp. 101-108.
  - Franja Šulek, Ingrid Milošev, "Inhibitory effects of chitosan coating against biofilm formation on metal implants", In: *Cross-border Italy-Slovenia biomedical research: are we ready for horizon 2020?: conference proceedings with an analysis of innovation management and knowledge transfer potential for a smart specialization strategy = atti della conferenza = zbornik*, Sabina Passamonti, ed., 1st printed ed., Trieste, Edizioni Università di Trieste, 2014, pp. 133-138.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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- Ingrid Milošev, Vesna Levašič, Andrej Cör, Venčeslav Pišot, "Mechanical, biological, material and clinical aspects of performance of joint prostheses", In: *The partners and the objectives of Trans2Care, an Italy-Slovenia cross-border network of science and healthcare institutions*, Sabina Passamonti, ed., 1st printed ed., Trieste, Edizioni Università di Trieste, 2014, pp. 105-108.
- Franja Šulek, Ingrid Milošev, "Nanocoatings for preventing orthopaedic implant-associated bacterial infections", In: *The partners and the objectives of Trans2Care, an Italy-Slovenia cross-border network of science and healthcare institutions*, Sabina Passamonti, ed., 1st printed ed., Trieste, Edizioni Università di Trieste, 2014, pp. 111-115.

## PATENT APPLICATION

- Peter Rodič, Ingrid Milošev, *Hybrid sol-gel compositions and corrosion-resistant coatings based upon same*, PCT/IB2014/062687, WIPO International Bureau, 27.6.2014.

## MENTORING

- Rok Prebil, *Aerobic oxidative transformations of organic compounds catalyzed by nitrates*: doctoral dissertation, Ljubljana, 2014 (mentor Stojan Stavber; co-mentor Marjan Jereb).
- Peter Rodič, *Corrosion protection of aluminium and aluminium alloys using hybrid sol-gel coatings*: doctoral dissertation, Ljubljana, 2014 (mentor Ingrid Milošev; co-mentor Boris Pihlar).
- Matevž Topolovec, *Influence of bearing surfaces on survivorship of total hip replacements*: doctoral dissertation, Ljubljana, 2014 (mentor Ingrid Milošev; co-mentor Andrej Cör).

## PUBLISHED CONFERENCE CONTRIBUTION

- Njomza Ajvazi, Stojan Stavber, "Comprehensive transformation of alcohols catalysed by N-halocompounds under solvent-free reaction conditions", In: *Slovenski kemijski dnevi 2014, Maribor, 11. - 12. september 2014, Slovenski kemijski dnevi 2014, Maribor, 11.-12. september 2014, Zdravko Kravanja, ed., Miloš Bogataj, ed., Zorka Novak-Pintarič, ed., Maribor, Fakulteta za kemijo in kemijsko tehnologijo, 2014, 8 pp.*



# ELECTRONIC CERAMICS DEPARTMENT

# K-5

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

In the framework of lead-free piezoelectric materials, we were particularly interested in alkali-niobate-based ceramics, which are still considered as one of the most important candidates for the replacement of lead-based perovskites in piezoelectric applications. In collaboration with the Montanuniversität Leoben, Austria, University of Nova Gorica, National Institute of Chemistry, Ljubljana, and University of Ljubljana we investigated the influence of strontium additions on the phase composition, microstructure and crystal structure of the  $K_{0.5}Na_{0.5}NbO_3$  (KNN) solid solution. By increasing the amount of strontium a decrease of the grain size, segregation of the secondary phase and a change of the KNN crystal structure from monoclinic to cubic symmetry were observed.

Within the activities on lead-based piezoelectric ceramics, in the frame of the 7FP EU project CERAMPOL and in collaboration with the company HIPOT-RR, we continued our study of the fabrication of waste-water cleaning systems. The system is based on the integration of piezoelectric  $Pb(Zr,Ti)O_3$  (PZT) actuators onto a porous ceramic substrate. With the support of the numerical modelling and vibration measurements of a substrate with integrated piezoelectric actuators, we defined the optimal geometry of the system. The vibration system was tested under real operating conditions by the project partners.

In collaboration with the Instituto de Ciencia de Materiales de Madrid, Spain, we prepared  $\langle 001 \rangle$  orientated  $0.675Pb(Mg_{1/3}Nb_{2/3})O_3-0.325PbTiO_3$  ceramics with a very high piezoelectric coefficient  $d_{33}$  of 950 pm/V.

Within the studies on multiferroic  $BiFeO_3$ , we focused on two systems, i.e.,  $BiFeO_3-SrTiO_3$  and  $BiFeO_3-REFeO_3$  (RE=Sm, Gd, Dy). We identified the key processing problem associated with the formation of Bi-rich secondary phases, which melted during the sintering and wetted the grains of the final ceramics. This problem was solved with two different approaches: i) by mechanochemical activation of the starting powder mixture, which resulted in an increased powder homogeneity, and ii) by performing the reaction using pre-synthesized  $BiFeO_3$  and  $SrTiO_3$  binaries, in which case we avoided the use of  $Bi_2O_3$  in the initial mixture and thus the formation of  $Bi_2O_3$ -rich phases with low melting points. We have also studied the processing of Sm-modified  $BiFeO_3$ . We found that during the reactive sintering the  $Sm_2O_3$  reacts preferentially with Si impurities without a large increase in the concentration of the Bi- and Fe-rich secondary phases, which are otherwise formed during the processing of unmodified  $BiFeO_3$  due to the reaction between the Si and the  $Bi_2O_3$ .

In 2014 we published a review article on piezoelectric  $BiFeO_3$  material entitled "BiFeO<sub>3</sub> Ceramics: Processing, Electrical, Electromechanical Properties." The article was published in the July issue of the "Journal of the American Ceramic Society" and had a cover picture produced by researchers from the K-5 department. (Figure 1)

In collaboration with the Department of Physics, University of Iasi, Romania, we systematically studied  $BaSn_xTi_{1-x}O_3$  ferroelectric-relaxor cross-over induced by an increase of the tin addition (to  $x=0.20$ ). The tin addition causes a gradual modification in the lamellar domain structure and by approaching the relaxor compositions ( $x = 0.15$  and  $0.20$ ) polar nano-regions become crucial in the behaviour of the low- and high-field dielectric properties of the materials.

We studied the electrocaloric (EC) response of  $PbZrO_3$  bulk ceramics together with colleagues from the Condensed Matter Physics Department at the JSI. The samples were prepared by sintering at a uniaxial pressure of 24.5 MPa and at 950 °C. By direct EC measurements the negative EC effect in this antiferroelectric ceramic was confirmed.



Head:  
**Prof. Barbara Malič**

**In collaboration with research groups from Switzerland, Australia and the USA we published a feature paper in the Journal of the American Ceramic Society entitled "BiFeO<sub>3</sub> ceramics: Processing, Electrical, and Electromechanical Properties". The review article presents the most important achievements of the department and other laboratories around the world in the field of BiFeO<sub>3</sub>, which has been the most studied perovskite over the past decade.**



Figure 1: Cover of the July issue of the "Journal of the American Ceramic Society", created by researchers from the K-5 department.



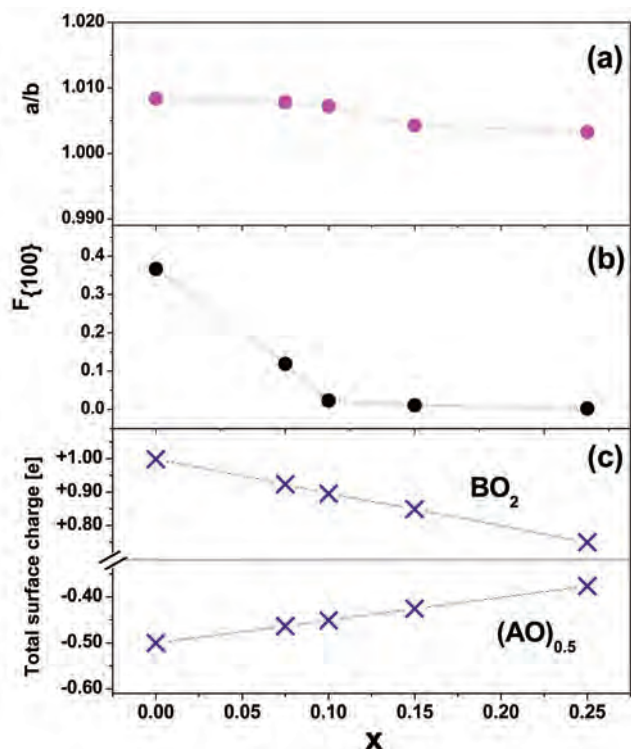


Figure 2: KNN and (1-x)KNN-xSTO thin films: a) ratio of a/b lattice parameters, b) Lotgering factor F{100} and c) the total surface charge of the individual atomic layers in the solid solution (A: K, Na, Sr; B: Nb, Ti).

**Dielectric thin films based on tantalum oxide, prepared by solution synthesis upon heating at as low as 300–350 °C, exhibit suitable electrical and optical properties for use as transparent passive or active electronic components.**

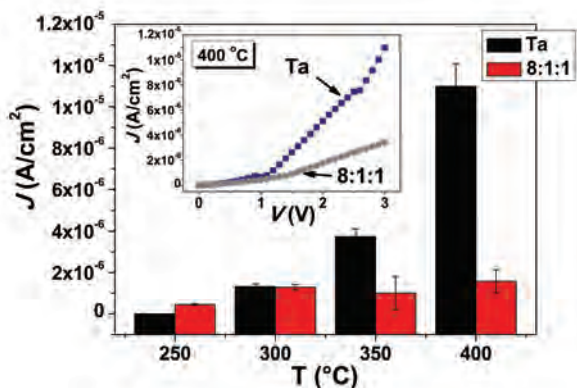


Figure 3: Leakage current density at an applied electric field of 160 kV/cm as a function of processing temperature of the Ta<sub>2</sub>O<sub>5</sub> (Ta) and 8:1:1 thin films. The inset shows the current density versus applied voltage for the samples processed at 400 °C.

Within studies of environment-friendly lead-free ferroelectric and relaxor thin films by chemical solution deposition, the focus was on the (1-x) K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub>-xSrTiO<sub>3</sub> solid solution (KNN-STO), x = 0.075–0.25. Thin films on platinised silicon substrates crystallize in a pure perovskite phase upon rapid thermal annealing at 750 °C for 5 minutes. By increasing the fraction of STO the monoclinic distortion, the volume of the unit cell, the grain size and the degree of preferential {100} orientation in the films decreased (Figure). The latter was connected to the differences in the average surface energies of the {100} crystal planes of the KNN and STO end-members. (Figure 2) The temperature of the dielectric permittivity maximum decreased with the increasing STO content in the films. In collaboration with colleagues from the Condensed Matter Physics Department the relaxor behaviour of the 0.85KNN–0.15STO thin films was confirmed by dielectric spectroscopy and polarization vs. electric field measurements.

We prepared thin-film varactors based on Ba<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> (x = 0.5, 0.4, 0.3) with partners from the Faculty of Electrical Engineering, University of Ljubljana, Experimental Particle Physics Department and Centre of Excellence SPACE.SI within the European Space Agency (ESA) JP PECS project FERROPATCH. The solution-derived films were deposited on polycrystalline alumina substrates and rapid thermally annealed at 900 °C. The in-plane microstructures of the about 240-nm-thin films were not much influenced by the change of the chemical composition, in all cases they were dense and consisted of about 100 nm grains. By increasing the fraction of Sr in the solid solution the dielectric permittivity and losses at 10 GHz decreased from 1310 and 0.142 to 670 and 0.024 for x = 0.5 and 0.3, respectively. Thus the solid solution with x = 0.3 was selected for the design and realization of a frequency and polarisation agile microwave antenna.

Within the 7FP EU project ORAMA we continued our work on transparent conducting oxides and dielectrics for transparent electronics. In collaboration with our partners from CNR-INO SENSOR Lab, University of Brescia, Italy, both p- and n-type Cu-Al-O thin films were deposited by RF magnetron sputtering from a single-phase CuAlO<sub>2</sub> target. It was shown that the p-type films could be used as innovative gas sensors for ozone detection, since their response towards 70 ppb of ozone was R = 100 at 300 °C and R=10 at 400 °C, i.e., two- and five-orders-of-magnitude higher than that reported for CuO and CuAlO<sub>2</sub> thin films at 300 °C, respectively.

We continued the research on high-K dielectric thin films based on Ta<sub>2</sub>O<sub>5</sub> and Ta<sub>2</sub>O<sub>5</sub>-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> in the 8:1:1 molar ratio (further denoted as 8:1:1) for transparent electronics together with colleagues from the Faculty of Electrical Engineering, University of Ljubljana. The solution-derived films were processed at temperatures not exceeding 400 °C. The leakage currents proved to be dependent on the thermal budget of the samples. The Ta<sub>2</sub>O<sub>5</sub> sample processed at 400 °C showed a leakage current density ( $J$ ) of 10<sup>-5</sup> A/cm<sup>2</sup> at 3V, i.e., at ~260 kV/cm, whereas the 8:1:1 sample exhibited almost an order of magnitude lower  $J$  value. However, the  $J$  values measured for both samples processed at 300 °C were in the range 1.4–2×10<sup>-6</sup> A/cm<sup>2</sup>. (Figure 3) Together with ORAMA project partners from Universidade Nova de Lisboa, Portugal, we verified whether the tantalum-oxide-based thin films processed at 300 and 350 °C, could be implemented as gate-dielectrics in thin-film transistors (TFTs). The TFTs on glass substrates with integrated dielectrics exhibited an on/off ratio > 10<sup>8</sup>. Therefore, both Ta<sub>2</sub>O<sub>5</sub> and 8:1:1 thin films from solution proved to be suitable for TFT applications.

In the framework of piezoelectric thick films, we dispersed lead-zirconate-titanate powder in ethanol and deposited it onto patterned strip electrodes by the electrophoretic deposition (EPD) process. By varying the deposition time, the distance between the electrodes and the geometry of the counter electrode we deposited about 1-mm-wide lines with a uniform

thickness and a distance between the lines of about 0.4 mm. The elements had about 85 % of theoretical density and were about 20- $\mu\text{m}$  thick after sintering at 950 °C. In collaboration with researchers from François-Rabelais University Tours, France, the elements were electromechanically characterized. They had a resonance frequency of around 70 MHz and a dielectric constant of around 370 and can be used for the fabrication of high-frequency linear-array transducers.

We continued the study of processing porous lead zirconate titanate (PZT) ceramics with controlled porosity, pore size and pore size distribution. By sintering the powder compacts with a homogeneous distribution of PZT and polymethyl methacrylate (PMMA) particles at selected temperatures we obtained ceramics with a porosity of about 30 % and a narrow pore size distribution with the pore sizes around 1 or 10  $\mu\text{m}$ . The ceramics possess a high attenuation coefficient and will be used as a backing for high-frequency ultrasound transducers.

Furthermore, we investigated the influence of the surface roughness of the platinum substrates on the functional properties of  $0.65\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.35\text{PbTiO}_3$  thick films. The thick-film pastes were screen-printed on the platinum substrates, which differed in the surface roughness by almost an order of magnitude; namely, vertical mean roughness (rms) values, determined by atomic force microscope, of 44 nm and 342 nm, respectively. The films on the flat substrates exhibited a higher degree of (001) orientation of the tetragonal phase, and a higher remnant polarization than the films on the rough substrates.

With colleagues from the Department for Condensed Matter Physics, JSI, we studied the electrocaloric (EC) response of the  $0.7\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3-0.3\text{PbTiO}_3$  thick films on platinum foils. The highest EC temperature change of 1.2 K was observed at 380 K and at an applied electric field of 120 kV/cm.

We prepared  $\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3-\text{Pb}_2\text{Ru}_2\text{O}_{6.5}$  (PZT-PRO) thick-film composite materials (with 10, 15, 20 and 25 vol % of PRO). The thick-film pastes were screen-printed and fired on sapphire substrates. In collaboration with colleagues from the Institute of Physics, Academy of Sciences, Czech Republic, we found that unlike the low-frequency permittivity, which diverges at the percolation threshold, near the composition with 17 vol% PRO, the THz and microwave permittivities increase even above the threshold value.

We studied the preparation, structural and microstructural properties of KNN thick films screen-printed on different substrates. By optimizing the synthesis conditions, particularly the sintering temperature, the amount of germanate-based liquid-phase sintering additive and the packing powder we successfully prepared single-phase, dense, crystallographically oriented KNN thick films. (Figure 4) By using high-temperature “in-situ” X-ray analysis we explained the mechanism of orientation as being due to the thermal expansion coefficients mismatch of the KNN and  $\text{Al}_2\text{O}_3$  substrate during cooling. The results raise the possibility of controlling the orientation and hence the functional properties of KNN thick films by the selection of the substrate.

We prepared  $\text{BiFeO}_3$  (BFO)/substrate thick-film structures by screen-printing and studied the influence of different substrates on the density, phase composition and structure of the films. We showed that the structure and phase composition of the BFO is strongly dependent on the annealing temperature and the impurities present in the substrate, which may even in small amounts react with BFO and form unwanted secondary phases.

We continued the investigations of LTCC (Low Temperature Co-fired Ceramics), which are used for the fabrication of 3D structures for different electromechanical (MEMS - Micro Electro Mechanical Systems) and chemical microsystems. Traditional cooperation with research partners from HIPOT-RR and Centre of Excellence NAMASTE continued in all research projects related to thick-film and LTCC technology, in particular, we developed the technological process for the integration of various functional elements, such as quartz glass, porous corundum ceramics or piezoelectric ceramics into the structure of LTCC.

In cooperation with the above-mentioned research partners, we designed and created various demonstrators based on LTCC material developed by the company KEKO Equipment d.o.o. An example of such a product is a micro-ozonator, which is composed of several LTCC layers with different dielectric properties.

With the group from the company KEKON d.o.o. we continued our research in the field of functional thick-film materials for multi-layered electronic components.

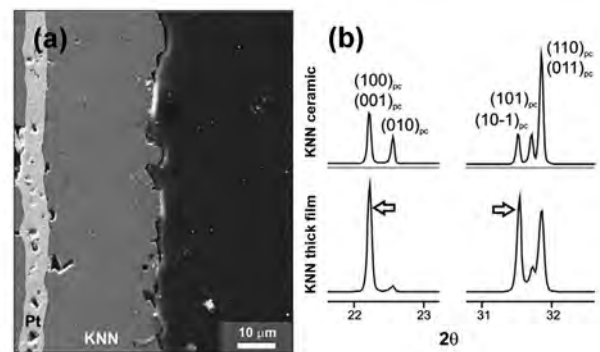


Figure 4: (a) Cross-section of a dense and single-phase KNN thick film with no visible defects. (b) X-ray patterns of KNN in thick-film and ceramic forms, showing the crystallographic orientation of the film (arrows), which was achieved by the appropriate selection of the substrate.

**We have prepared functional thin and thick films of environmentally friendly ferroelectrics based on  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$ .**



Figure 5: Researchers from the K-5 department in cooperation with ETI d.d. from Izlake received the Silver Award for Innovation "New cordierite material C 410 for electrical engineering and its process for manufacturing"

In collaboration with the company ETI Elektroelement d.d. from Izlake we developed a new C410 type of cordierite material that is used in electrical engineering as a heat or electrical insulator. The cordierite ceramic is fabricated from numerous natural raw materials. Since the properties of raw materials may vary from batch to batch it is difficult to fabricate products with reproducible properties. By optimising the number of raw materials and their quantities, we developed a new material with the required flexural strength and thermal expansion coefficient. The low-priced material enables the fabrication of products with reproducible properties and is used in mass production in the company. The researchers from the K-5 department and ETI Elektroelement, d. d., received for this invention the Silver Award for innovation "New cordierite material C 410 for electrical engineering and its process for manufacturing", by Regional Chamber of Commerce of Zasavje, in June 2014 (Figure 5).

### Some outstanding publications in the past year

1. Rojac, T., Benčan, A., Malič, B., Tutuncu, G., Jones, J. L., Daniels, J. E., Damjanović, D.: BiFeO<sub>3</sub> ceramics : processing, electrical, and electromechanical properties. *Journal of the American Ceramic Society*, ISSN 0002-7820, 2014, 97 [7], 1993–2011
2. Koruza, J., Malič, B.: Initial stage sintering mechanism of NaNbO<sub>3</sub> and implications regarding the densification of alkaline niobates. *Journal of the European ceramic society*, ISSN 0955-2219, 2014, 34 [ 8], 1971–1979
3. Frunza, R. C., Kmet, B., Jankovec, M., Topič, M., Malič, B.: Ta<sub>2</sub>O<sub>5</sub>-based high-K dielectric thin films from solution processed at low temperatures. *Materials research bulletin*, ISSN 0025-5408, 2014, 50, 323–328
4. Pavlič, J., Malič, B., Rojac, T.: Microstructural, structural, dielectric and piezoelectric properties of potassium sodium niobate thick films. *Journal of the European ceramic society*, ISSN 0955-2219, 2014, 34 [2], 285–295
5. Noshchenko, O., Kuščer, D., Mocioiu, O. C., Zaharescu, M., Bele, M., Malič, B.: Effect of milling time and pH on the dispersibility of lead zirconate titanate in aqueous media for inkjet printing. *Journal of the European ceramic society*, 2014, 34 [2], 297–305

### Awards and appointments

1. Ines Bantan, Janez Holc, Danjela Kuščer, Joži Prašnikar, Helena Razpotnik: Silver acknowledgment for the inovation, Chamber of Commerce and Industry of Slovenia, Zagorje ob Savi, New Cordierite material C410 for the electrotechnics and the procedure of its fabrication
2. Hana Uršič Nemevšek: Award at the conference COST MP0904 Action, Bucharest, Romania, Internal Advisory Board of the COST Single- and multiphase ferroics and multiferroics with restricted geometries (SIMUFER), Unusual structural-disorder behavior of Pb(Sc<sub>0.5</sub>Nb<sub>0.5</sub>)O<sub>3</sub>
3. Jitka Hreščak: Acknowledgement for the presentation of the research achievements from the view of science quality and their usefulness: Ljubljana, Jožef Stefan International Postgraduate School, The role of different niobium pentoxide precursors in the solid-state synthesis of potassium sodium niobate
4. Julian Walker: Excellence Award for the Best Oral Presentation of young scientist, Ekaterinburg, Russian Federation, Organizational Board of the Joint International Conference Piezoresponse Force Microscopy and Nanoscale Phenomena in Polar Materials, Electrical, electromechanical properties and domain structure of Sm-modified-BiFeO<sub>3</sub> ceramics prepared by mechanochemical activation

## INTERNATIONAL PROJECTS

1. 7FP - ORAMA; Oxide Materials Towards a Matured Post-silicon Electronics Era  
Prof. Barbara Malič  
European Commission
2. 7FP - CERAMPOL; Ceramic and Polymeric Membrane for Water Purification of Heavy Metal and Hazardous Organic Compound  
Asst. Prof. Danjela Kuščer Hrovatin  
European Commission
3. 7FP - PI; The Piezo Institute - European Expertise Centre for Multifunctional and Integrated Piezoelectric Devices  
Prof. Barbara Malič  
European Commission
4. FERRO-PATCH; Frequency and Polarisation Agile Microstrip Patch Antenna based on Ferrelectric Varactors  
Prof. Barbara Malič  
ESA/ESTEC.
5. COST MP0904; SIMUFER: Single- and Multiphase Ferroics and Multiferroics with Restricted Geometries  
Prof. Barbara Malič  
COST Office

6. COST MP1308; Towards Oxide Based Electronics  
Dr. Katarina Vojisavljević  
COST Office
7. Study on the Process and Mechanism of Novel Electronic Ceramics  
Prof. Barbara Malič  
Slovenian Research Agency
8. Multiferroic Composites for Novel Applications  
Asst. Prof. Andreja Benčan Golob  
Slovenian Research Agency
9. Processing-properties Relationship in Lead-free (K,Na)NbO<sub>3</sub>-based Piezoelectric Materials  
Asst. Prof. Tadej Rojac  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Electronic Ceramics, Nano-, 2D and 3D Structures  
Prof. Barbara Malič



## R & D GRANTS AND CONTRACTS

- Oxide-based Components for Transparent Electronics  
Prof. Barbara Malič
- Nanostructures for High-efficiency Solar Cells and Photovoltaic  
Prof. Barbara Malič
- Tunable Ferroelectric Thin Film Capacitors for Agile Microwave Antennas  
Prof. Barbara Malič
- High-performance Piezoelectric Materials for Sensors and Actuators in High-temperature Applications  
Asst. Prof. Tadej Rojac
- New Advanced Electrocaloric Materials for Novel Environmentally Friendly Dielectric Refrigeration Technology  
Prof. Barbara Malič
- Materials and Technologies for Chemical Microsystems  
Asst. Prof. Andreja Benčan Golob

- Micro-electromechanical and Electrocaloric Layer Elements  
Prof. Barbara Malič
- Processing of Stable Aqueous Suspensions for Fabrication of Electrotechnical Elements based on Steatite Ceramic  
Dr. Katja Makovšek

## NEW CONTRACTS

- Research of Steatite Materials C220, C221, C230  
Asst. Prof. Danjela Kuščer Hrovatin  
Development Centre RC eNeM, Ltd.
- Research of Cordierite Materials C410, C520, C530  
Prof. Barbara Malič  
Development Centre RC eNeM, Ltd.

## VISITORS FROM ABROAD

- Naonori Sakamoto, Department of Electronics and Materials Science, Shizuoka University, Shizuoka, Japan, 13 March–13 September 2014
- Andreas Klein, Technische Universität Darmstadt, Institute for Materials Science, Darmstadt, Germany, 12–15 March 2014
- Nadia El Fels, Université de Limoges, Faculté des Sciences et Techniques, Limoges, France, 7 April–13 July 2014
- Maria Zaharescu, "Ilie Murgulescu" Institute of Physical Chemistry of Romanian Academy, Bucharest, Romania, 6–8 April 2014
- Mahdi Feizpour, Ceramics Division-Materials and Energy Research Center, Meshkin-dasht, Karaj, Alborz, Iran, 15 July–15 December 2014
- Dragan Damjanović, Ceramics Laboratory, Swiss Federal Institute for Technology-EPFL, Lausanne, Switzerland, 23–26 June 2014
- Andre-Pierre Abellard, Université François Rabelais, Tours, France, 19–26 June 2014
- Tomoya Ohno, Kitami Institute of Technology, Kitami, Japan, 21–24 June 2014
- Takashi Arai, Kitami Institute of Technology, Kitami, Japan, 21–24 June 2014
- Garry L. Messing, Penn State University, Penn State, USA, 4–5 June 2014
- John Daniels, School of Materials Science and Engineering, UNSW Australia, Sydney, Australia, 21–23 September 2014
- Leszek Golonka, Faculty of Microsystem Electronics and Photonics, Wrocław University of Technology, Wrocław, Poland, 7–10 October 2014
- Vincenzo Buscaglia, National Research Council, Institute for Energetics and Interphases IENI, Genova, Italy, 22–24 October 2014
- Andrei Kholkin, Ural Federal University, Ekaterinburg, Russian Federation, 11–14 December 2014

## STAFF

### Researchers

- Asst. Prof. Andreja Benčan Golob
- Asst. Prof. Goran Dražić\*
- Asst. Prof. Marko Hrovat, retired 01. 08. 14
- Asst. Prof. Danjela Kuščer Hrovatin
- Prof. Barbara Malič, Head**
- Asst. Prof. Tadej Rojac
- Dr. Marina Santo Zarnik\*
- Dr. Hana Uršič Nemevšek

### Postdoctoral associates

- Dr. Georgia Basina, left 15. 05. 14
- Dr. Mara Bernardo Sacristan
- Dr. Alja Kupec
- Dr. Kostja Makarovič\*
- Dr. Katja Makovšek
- Dr. Brigita Rožič, left 01. 02. 14
- Dr. Katarina Vojsavljević
- Dr. Julian Bradley Walker

### Postgraduates

- Tina Bakarič, B. Sc.
- Raluca-Camelia Frunza, B. Sc.

- Lovro Fulanović, B. Sc.
- Jitka Hřešćak, B. Sc.
- Evgeniya Khomyakova, B. Sc.
- Dr. Oleksandr Noshchenko, left 01. 05. 14
- Jernej Pavlič, B. Sc.
- Tanja Pečnik, B. Sc.
- Jerca Praprotnik, B. Sc., left 01. 09. 14
- Marko Vrabelj, B. Sc.
- Technical officers**
- Darko Belavič, B. Sc.
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# ENGINEERING CERAMICS DEPARTMENT

# K-6

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

The investigation of AlN powder hydrolysis in diluted aqueous suspensions was continued in 2014. A diploma thesis entitled “*Processing of high-performance nanocomposite ceramics  $ZrO_2 - Al_2O_3$  (ATZ)*” was completed. In this work a high-performance ATZ nanocomposite, differing in alumina ( $Al_2O_3$ ) content, was prepared and characterized. For this purpose an ATZ powder precursor was synthesized by exploiting the hydrolysis of AlN powder. Specimens were consolidated and sintered by using a modern sintering technique, known as spark-plasma sintering (SPS), based on the pulsed-current activated sintering under uniaxial pressing and vacuum. By using SPS, we have managed to reduce the  $ZrO_2$  crystal grain size by 3-times, compared to the conventional sintering (and in the literature). We have managed to keep  $Al_2O_3$  particles in the nanoscale regime (less than 100 nm), which were homogeneously distributed at triple junctions in the  $ZrO_2$  matrix. Moreover, a minor fraction of intragranular  $Al_2O_3$  nanoparticles of even smaller size (30–50 nm) within the  $ZrO_2$  grains contributed to the enhanced mechanical properties of the ATZ nanocomposites.

The research in the field of electrically conductive ceramic composites based on zirconia (Y-TZP) with dispersed titanium nitride (TiN) particles that could be machined with electrical-discharge machining was continued. Homogeneous powder mixtures  $ZrO_2/TiN$  with various amounts of TiN were prepared by the controlled, in-situ precipitation of titanium oxide on the surfaces of zirconia particles, which was followed by calcination and a thermochemical treatment in ammonia (nitridation) to yield titanium nitride. These were consolidated using the spark-plasma sintering (SPS) technique to produce dense composites. The impact of the content and the size of the conductive particles on the densification process and the final mechanical and electrical properties of the composites were studied. Using electron microscopy it was confirmed that upon densification, electrically conductive TiN particles retained their nanometre size and as a consequence the materials containing only 13 vol.% of TiN exhibited a sufficiently high electrical conductivity for machining using EDM.

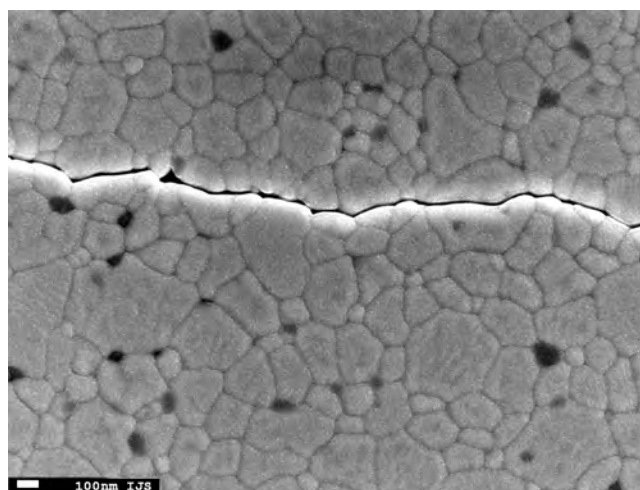
The research on the synthesis of electrically conductive ceramic composites based on silicon nitride ( $Si_3N_4$ ) was resumed by taking advantage of the SPS technique in the densification of  $Si_3N_4$  powders coated with TiN or ZrN nanoparticles. Very high heating rates and fast densification compared to conventional sintering hindered the excessive growth of the conductive nanoparticles, which was not possible before. Also in this case, the electrically conductive composites with a smaller amount of conductive phase (under 15 vol.%) were successfully prepared.

In 2014 the research on self-healing ceramic composites based on silicon nitride/silicon carbide composites was continued. The  $Si_3N_4$  matrix with dispersed SiC nanoparticles was prepared by mixing the  $Si_3N_4$  powder with a polycarbosilane polymeric ceramic precursor, which forms SiC after pyrolysis. The powder mixtures containing different amounts of SiC were successfully densified using SPS, while the size of the SiC particles remained on the nanoscale. These materials exhibit better oxidation resistance and mechanical properties compared to conventionally prepared  $Si_3N_4/SiC$  composites. It was also demonstrated that the surface cracks made by the



Head:  
**Prof. Tomaž Kosmač**

**Dr Andraž Kocjan was one of the co-authors of the article “Thermally insulating and fire-retardant lightweight anisotropic foams based on nanocellulose and graphene oxide” that was published in the journal Nature Nanotechnology.**



*Figure 1: SEM micrograph of ATZ nanocomposite microstructure, where homogeneously distributed  $Al_2O_3$  nanoparticles reside at triple junctions and even within the grains of the  $ZrO_2$  matrix.  $Al_2O_3$  nanoparticles contribute to enhanced crack deflection, induced by a Vickers prism.*



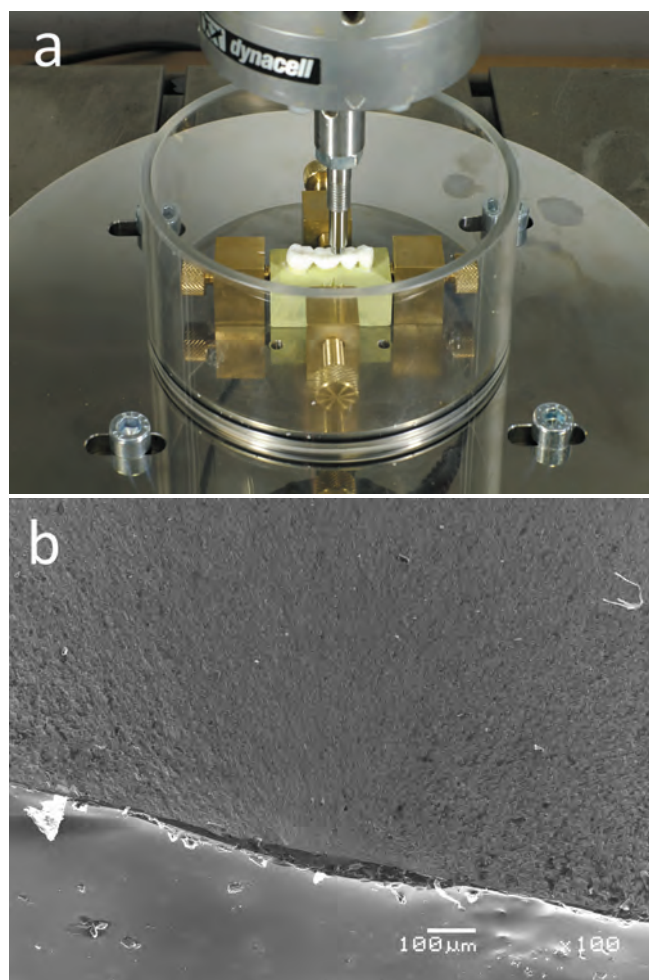


Figure 2: Setup for the mechanical loading of the FPDs in a moist environment (a) and an image of the fracture surface of an FPD (the fracture origin and direction of the crack propagation are indicated) (b).

Vickers indentation can be closed during the oxidation treatment, indicating a possible self-healing ability.

In the field of research on dental ceramics we continued addressing some of the major problems concerning the production of full-ceramic dental dentures with tetragonal zirconia (Y-TZP) as a core material, their cementation and their behaviour in clinical conditions. The work was conducted in close cooperation with the Department of Oral Medicine, Medical Faculty at the University of Ljubljana. Thus, extensive *in-vitro* experiments were conducted aimed at a better understanding of the ageing process, i.e., the hydrothermally induced transformation of the metastable tetragonal zirconia into the thermodynamically stable monoclinic structure. This transformation is accompanied by micro-cracking, which ultimately leads to strength degradation. In order to elucidate the role of phase partitioning occurring within the individual grains during sintering, three materials exhibiting nearly the same grain size distribution were produced under different sintering conditions resulting in different amounts of transformable (tetragonal) and untransformable (cubic) zirconia. It was found that the material that was sintered for a longer period of time at a lower temperature contained a larger amount of cubic zirconia and consequently aged at a significantly higher rate compared to the material sintered for a shorter period at a higher temperature. Also, as part of a PhD thesis, the combined effects of silica and alumina on the ageing resistance and mechanical properties of 3Y-TZP ceramics were investigated. The specimens were prepared by the infiltration of a silica sol into the pre-sintered porous 3Y-TZP pellets, produced from commercially available powders, containing different amounts of alumina (0.05 and 0.25 wt. %). It was found that the presence of silica in alumina-free 3Y-TZP greatly increases the resistance to ageing. The addition of small amounts of silica to alumina-containing 3Y-TZP further improves the ageing properties of the t-zirconia, in part due to a possible distinctive mechanism of suppression, and in another part due to a strong effect of dopants on the phase partitioning. In addition to these *in-vitro* experiments, an *in-vivo* study has been continued aimed at monitoring the propagation of the t-m transformation of “high-translucency” 3Y-TZP ceramics directly exposed to the aggressive environment of the oral cavity in the absence of an externally

applied stress. In this experiment, sintered zirconia discs differing in their composition, microstructure and surface treatment, were implanted in the lingual flange of the lower dentures to be worn by recruited edentulous patients from the Department of Prosthodontics, Medical Faculty, University of Ljubljana. After every 6 months the discs are being explanted, gently cleaned by ultrasonication to remove the adhered proteins, and subjected to XRD and FE-SEM surface analyses. Yet another clinical testing was started in 2013, involving the surface functionalization of sintered zirconia by applying nanostructured adhesive coatings in a non-invasive process that has been recently developed in our group. Two types of dentures were deemed to be most appropriate for the verification of nanostructured adhesive coatings in practice: three-unit inlay-retained bridges replacing missing single premolars and molars that have become increasingly popular due to the conservative approach to prosthetic rehabilitation, and conical primary crowns supporting secondary galvano-crowns of removable partial dentures. Finally, the first part of an extensive *in-vitro* study designed at evaluating the durability and reliability of “high translucent” full-anatomic, four-unit, posterior bridges was accomplished that involved accelerated ageing and mechanical fatigue testing under simulated clinical conditions. We were interested in compromise solutions between the aesthetic design (thickness of the abutments and their transition to connectors) and the durability for materials differing in sintering conditions and surface treatment.

In 2014, Dr Andraž Kocjan was involved in a collaboration of an international group of scientists from distinguished institutions including Stockholm University, Institute of Materials Science of Madrid, Instituto Politécnico de Torino and Max Planck Institute (Potsdam) that developed a new foam-like composite material that could dramatically reduce the cost of the heat insulation of buildings with a high energy efficiency. These foams, prepared by freeze-casting, exhibit a lower thermal conductivity than air and other commercially available, heat-insulating materials. For an example, unlike standard thermally insulating materials, i.e., polystyrene foam (EPS; polystyrene), where the addition of toxic halogenated compounds is necessary in order to improve the flame resistance, and silica aerogels, which are very brittle, the newly prepared foams with no hazardous additives are fire-retardant, ultra-light

and mechanically strong. In addition to all these technological advantages, resulting from a synergistic combination of structure and used components, the newly prepared foams from naturally abundant and renewable materials could lead to an important step within the sustainable development of the thermal insulation of buildings. The study, entitled “*Thermally insulating and fire-retardant lightweight anisotropic foams based on nanocellulose and graphene oxide*” was published in the renowned scientific journal Nature Nanotechnology. In this study, Dr Andraž Kocjan characterized the thermal properties of these composite foams using the equipment acquired via the Centre of Excellence NAMASTE, and discussed the obtained results.

Dr Andraž Kocjan also finalized and submitted for publication yet another manuscript connected to his recent JECS Trust founded post-doctoral project entitled “*Improved Reliability of Translucent Dental Zirconia and Alumina Ceramics*”. The work was done at Stockholm University during the period 2011–2013. In the meantime, the project was successfully concluded, while the above-mentioned investigation on, “*Processing of zirconia nanoceramics from a coarse powder*”, was accepted for publication in 2014 and published at the beginning of 2015 in the *Journal of European Ceramic Society*.

With the publication of the article “*Synthesis of bioactive  $\beta$ -TCP coatings with tailored physico-chemical properties on zirconia bioceramics*” in the Journal of Material Science: Materials in Medicine the research on the synthesis of bioactive calcium phosphate coatings on zirconia (Y-TZP) ceramics was successfully completed. The coatings were prepared using a biomimetic method in which the ceramic substrate is immersed in a solution with the same physiological temperature and similar composition as human-blood plasma. In this article a new process for the synthesis of thin  $\beta$ -tricalcium phosphate coatings with very good mechanical properties is described. Mechanical tests showed that the adhesion of such coatings is comparable or even better than the adhesion of calcium phosphate coatings on commercially available bone grafts.

For INTERSOCKS, tovarna nogavic, d.o.o., a study was conducted, where we have analysed a special fabric with incorporated ceramic particles. For the analyses, scanning electron microscopy, X-ray diffraction and a thermographic camera were employed. For the CETIS company we analysed the thermal properties of sensors.

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**In 2014 we cooperated with research institutions and industrial partners.**

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### Some outstanding publications in the past three years

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2. Samodurova, A., Kocjan, A., Swain, M., Kosmač, T.: The combined effect of alumina and silica co-doping on the ageing resistance of 3Y-TZP bioceramics. *Acta materialia*, ISSN 1359-6454. [Print ed.], [in press] 2014, 11 pgs., doi: 10.1016/j.actbio.2014.09.009
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6. Gorjan, L., Kosmač, T., Dakskobler, A.: Single-step wick-debinding and sintering for powder injection molding. *Ceram. Int.* 2014 (available on-line 2013), vol. 40, issue 1, 887-891
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## INTERNATIONAL PROJECTS

1. Services  
Prof. Tomaž Kosmač  
Foreign buyers
2. 7FP - CERAMPOL; Ceramic and Polymeric Membrane for Water Purification of Heavy Metal and Hazardous Organic Compound  
Prof. Tomaž Kosmač  
European Commission
3. COST MP1301; NEWGEN, New Generation Biomimetic and Customized Implants for Bone Engineering  
Prof. Tomaž Kosmač  
COST Office

## RESEARCH PROGRAM

1. Engineering and Bio-ceramics  
Prof. Tomaž Kosmač

## R & D GRANTS AND CONTRACTS

1. Research of Dental Ceramics  
Prof. Tomaž Kosmač

## VISITOR FROM ABROAD

1. Dr. Dušan Bučevac, Department of Materials Science, Vinca Institute of Nuclear Sciences, Belgrade, Serbia, 1 September-31 December 2014

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  9. Tomislav Pustotnik

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## ORIGINAL ARTICLE

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2. Joško Valentinčič, Kristoffer Krnel, Ana Lazar, Andrej Lebar, "Machining of Y-TZP ceramic composites with reduced amount of conductive phase by EDM", In: *Conference proceedings*, 9th International Conference on Industrial Tools and Material Processing Technologies [also] ICIT & MPT, Ljubljana, Slovenia, April 9th - 11th 2014, Aleš Hančič, ed., et al, Celje, TECOS, Slovenian Tool and Die Development Centre, 2014, pp. 371-375.



# 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 the 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.*



Head:  
**Prof. Spomenka Kobe**

2014 was the second year of the EU FP7 project “Nanocrystalline permanent magnets based on hybrid metal-ferrites” (NANOPYME). Because Sr-ferrite particles prepared via high-energy ball milling did not exhibit sufficiently high magnetic properties, a hydrothermal synthesis was implemented. Furthermore, hydrothermally synthesized Sr-ferrite particles were used for the preparation of hard-soft magnetic composites. Such composites are particularly interesting due to the possibility of an exchange-coupling interaction between the phases, which leads to an increase in the maximum energy product of the magnet. The increase of latter in ferrite-based magnets is also one of the goals of the project.

In this year we finished our study on the effect of coatings on Sm–Co magnets to improve the corrosion resistance. We coated Sm–Co magnets using two technologies: standard galvanic nickel, and PVD sputtering (TiN, CrN or TiAlN). A combination of both was tried as well (galvanic and PVD), with bare magnets being used as a reference. The oxidation resistance was tested in air at three different temperatures (350, 450 and 550 °C). By periodical weighing of the magnets during annealing we were able to follow the progress of the oxidation, and finally extract the parabolic oxidation coefficients. All the coatings improved the oxidation resistance, with the best performance observed for the Ni/CrN combination. These results were confirmed by optical and scanning electron microscopy observations. Before and after the annealing experiments, the magnetic properties were measured too, showing that the magnetic properties deteriorate more slowly when coated.

In the scope of the European project Replacement and Original Magnet Engineering Options ROMEO one of the tasks is to produce a prototype electromotor based on Nd–Fe–B permanent magnets. A crucial demand of such magnets is to meet the stringent requirements of the industrial partners, which will build the prototype (VALEO, SIEMENS and DAIMLER).

The architecture of the magnets needs to be designed in such a way that the outer part of the magnets is more resistant to the demagnetizing field to which the magnets are exposed during the motor-operation at high-loads.

Goal 1 of the project is to achieve ambitious magnetic properties: a coercivity of 2000 kA/m or more and a remanence of at least 1.3 T at room temperature.

The Nd–Fe–B magnets need to be a representative of the family with a reduced amount of heavy rare earths (HREs). i.e., Dy and Tb. This means that the sintered magnets produced only via a conventional powder metallurgy process are not capable of achieving low concentrations of HRE and retain the magnetic properties at the extreme level of Goal 1.

Within the scope of the EU project ROMEO we also developed **highly coercive ( $H_{ci}$ ) isotropic permanent Nd–Fe–B-based magnets**. The high  $H_{ci}$  was achieved by addition of  $DyF_3$  suspension to commercially available MQU-F rapidly quenched ribbons. The ribbons were coated with  $DyF_3$  in isopropanol, spark plasma sintered and heat treated. The highest  $H_{ci}$  enhancement was obtained at 2.2 wt.% Dy-fraction, i.e., from 1580 to 2025 kA/m, which is a 25 % improvement. To understand the diffusion process of Dy into the Nd–Fe–B ribbons we performed micro-structural and chemical analysis of the high  $H_{ci}$  ribbons, using scanning (SEM) and transmission (TEM) electron microscopy. The EDXS-TEM mapping of nano-sized grains showed that the samples prior to the heat treatment do not contain Dy. After the heat-treatment process the Dy diffuses into the grains and forms core-shell-like structures,

**Post-sintering technology, developed at the Department for Nanostructured Materials was the only proposed technology that was able to satisfy all of the required conditions at once. It is called the grain-boundary diffusion process (GBDP), based on the electrophoretic deposition (EPD) of  $TbF_3$  powder. The process optimization was focused on temperature/time modification, which revealed the optimum temperature at 875°C for 10 h. Calculated values for the coercivity and the remanence of the GBDP magnets at room temperature were 2027 kA/m and 1.31 T. With these achievements, the main goal was achieved and the industrial partners will build a demonstrator on the basis of our technology.**



which are crucial for the major increase in  $H_{ci}$ . Further research will be based on a quantitative EELS-TEM analysis of samples before and after the heat treatment.

Within the 7th EU FP we coordinate another international research project called “Mag-Drive”, the aim of which is the development of new technologies for the production of rare-earth-based permanent magnets for high-efficiency electro-motor applications. Besides the coordination, our tasks in the project are spark-plasma sintering and microstructural and magnetic characterization of the samples.

**Nanostructured materials** based on Fe–Pd, Co–Pt and Fe–Pt exhibit unique properties, depending on their crystal structure and size, applicable in bio-sensing, actuation, cell separation or targeted drug delivery and advanced

cancer treatments. Electrochemical synthesis was applied for the processing of Fe–Pd and Co–Pt nanowires, where a kinetic study revealed the systems properties can be tailored with high reproducibility. Single Fe–Pd nanowires were investigated using magnetic force microscopy and the magnetization reversal mechanism study revealed the dominant contribution of the shape anisotropy and a square like hysteresis behaviour typical for magnetic mono-domain nanostructures. We have to emphasize that the magnetic properties of a single magnetic nanostructure is, due to its low volume and low magnetic signal, challenging to measure, and that these measurements represent an excellent basis for the magnetic nanostructures applications. Fe–Pd nanowires were successfully transformed into highly coercive tetragonal or  $L1_0$  phase with the highest coercivities achieved for this system. In Co–Pt nanowires, it was discovered that the crystallographic orientation of both phases texture, such that the  $[00-1]$  of the hcp phase and the  $[111]$  of the fcc phase are pointing almost perpendicular to the nanowire axis.

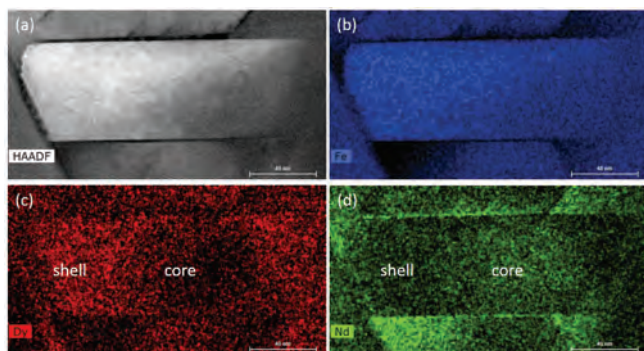


Figure 1 : EDXS-TEM mapping of Dy-treated Nd-Fe-B grain (a). Figure shows Fe (b), Nd (c) and Dy (d) maps, where Dy forms (Dy,Nd)-Fe-B shell around Nd-Fe-B core matrix.

The fitting of the experiment to these calculations results in a transverse effective anisotropy constant ( $K_{eff} = 2.6 \times 10^4 \text{ J/m}^3$ ) in the nanowires, which can be ascribed to the strong magnetocrystalline anisotropy of the hcp phase. A MFM study revealed that a spatial magnetization modulation was found to be length dependent. In order to correlate the magnetization distribution in nanostructures, we have started with modelling in order to investigate the magnetization distribution aspects and to translate theory into practice.

We have continued the work on multifunctional Fe–Pt– $\text{SiO}_2$ –Au core/shell nanoparticles (NPs) suitable for novel magneto-photo medical curing. The Fe–Pt nanoparticles were produced in a single and multicore version with improved magnetic properties, without affecting their superparamagnetic nature necessary for biomedical usage. Fe–Pt– $\text{SiO}_2$  NPs were further functionalized with biocompatible zwitterionic catechol ligands which introduce excellent hydrophilicity. Fe–Pt NPs were coated with  $\text{SiO}_2$ /Au and show large absorption the range between 550 and 850 nm, which make them superior to commercially available Au NPs with a discrete absorption peak. The suspension of these Fe–Pt– $\text{SiO}_2$ –Au core/shell nanoparticles was irradiated with a laser at the wavelength  $\lambda = 810 \text{ nm}$  at  $P = 1 \text{ W}$ . The temperature increased with a rate of 2 K/min, which makes this material suitable for photo thermal cancer treatments.

We investigated the isotropic-strain influence on magnetic ordering in systems with strongly-correlated 4f electrons of rare-earth elements. We demonstrated the relation between the topology of the Fermi surface and the type of magnetic ground state. Within the framework of the density-functional theory we explored the existence of magnetic phases in the system  $\text{Ca}_x\text{Gd}_{1-x}\text{Cu}_5$ . We determined the magnitude of the magneto-elastic coupling of the geometrically-frustrated ferromagnet  $\text{NaMnO}_2$ .

In 2014 the European programme EUROfusion (Horizon 2020) has been established. The department is involved with two projects aimed at the development of structural materials for the demonstration fusion reactor DEMO. In the project within the “Enabling research” we continued the development of the ceramic-matrix composite ( $\text{SiC}_f/\text{SiC}$ ). The second project (WPMAT) was focused on tungsten-based composites, where the goal is to improve the mechanical properties of tungsten under operational conditions by the addition of nanoparticles and/or fibres. The research has been partly performed in collaboration with the UK company TISICS Ltd.

In the final year of the project BioTiNet (FP7-ITN) we performed the last part of the study of nanocrystalline titania coatings applied to Ti-based alloys using a hydrothermal treatment of the alloy. Previous studies have confirmed the improved physico-chemical properties of the coatings as well as their beneficial interaction with proteins and human adipose cells. In the further study, performed in collaboration with Biotechnical Faculty, University of Ljubljana, and the Faculty for Mechanical Engineering, University of Ljubljana, *E-Coli* was used as a model system. The main goal was to understand the effects of surface charge, wetting and micro-roughness on the adhesion of bacteria. Using the specific hydrothermal treatment we succeeded in reducing the adhesion by 40 %, which attracted the attention of the producers of Ti-based biomaterials.

In the frame of the COST Action **Namabio** (From nano to macro biomaterials and applications to stem cells regenerative orthopaedic and dental medicine), the research of materials for tissue engineering has been continued. The research work has been aimed at the development of 3-dimensional biodegradable and bioactive scaffolds with bioactive glass for the osteochondral implants. We studied the effect of the bioactive glass nanoparticles embedded into gellan gum or a silk fibroin matrix on hydroxiapatite formation, biodegradability and the mechanical properties of the composite material. In collaboration with the Educell and Animacell (SMEs) we also started with the cell tests. In collaboration with the Spanish group CIDETEC we have also confirmed ability to prepare injectable bioactive scaffolds.

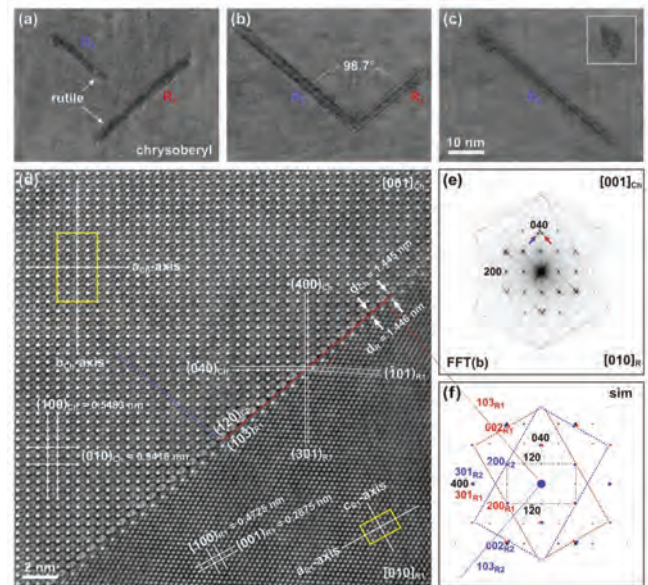
In the field of **photocatalysis** we designed and assembled various (micro)reactors based on photocatalytic titanium dioxide for chemical oxygen demand (COD) measurements in water in order to determine the overall content of organic compounds, as well as for the decomposition of the specific organic pollutants in water. The active part of a (micro)reactor is made of TiO<sub>2</sub> anatase nanotubes that are prepared by the anodic oxidation of titanium foil. The specific design of the photocatalytic reactor was protected by a patent.

Within the investigations of n-type oxide **thermoelectric materials** we synthesized Nb-doped SrTiO<sub>3</sub>. The basic microstructure of the solid solution Sr(Ti<sub>0.8</sub>Nb<sub>0.2</sub>)O<sub>3-x</sub> was modified with the addition of Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub> nucleation seeds and/or with the addition of SrO-excess. The Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub> seeds were synthesized using a molten-salt approach. In the case when the Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub> seeds were added to a Sr(Ti<sub>0.8</sub>Nb<sub>0.2</sub>)O<sub>3-x</sub> solid solution we were able to improve the thermoelectric properties of the material due to the lower thermal conductivity and the increased electrical conductivity. The figure of merit ZT thus increased from 0.09 to 0.14. By using high-resolution STEM HAADF imaging we were able to determine the Nb content on the B sites in the Sr(Ti<sub>0.8</sub>Nb<sub>0.2</sub>)O<sub>3-x</sub> solid solution with the perovskite structure.

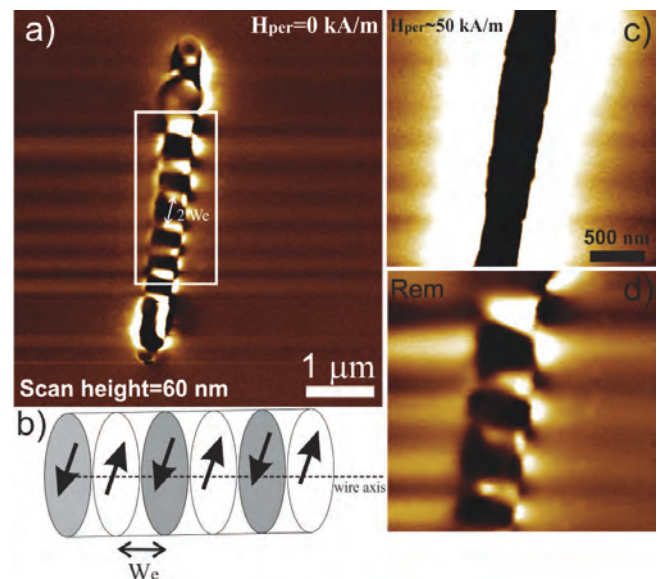
**Perovskite materials** such as BaTiO<sub>3</sub> and Fe-SrTiO<sub>3</sub> nanostructures are suitable for many applications, such as humidity or oxygen sensing and tunable HTS (high temperature superconducting) microwave filters. The potential advantages of the nanostructured forms have been, however, scarcely explored compared to other oxides. The synthesis of perovskite nanostructures via sol-gel electrophoretic deposition (EPD) into anodic aluminium oxide (AAO) membranes has proven to be very successful and useful. In the last year we submitted a postdoc project that was granted in the middle of the year. The project entitled "From the synthesis of metal oxides to the humidity and oxygen prototype nanosensors" focuses on the synthesis and gas-sensing device formation of the one-dimensional (1D) metal oxide nanostructures such as BaTiO<sub>3</sub>, Fe-doped SrTiO<sub>3</sub> and Y-doped ZrO<sub>2</sub> nanostructures.

We developed homogeneous coarse-grained low-voltage ZnO-based **varistor ceramics** doped with Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> or Bi<sub>12</sub>TiO<sub>20</sub> and other varistor dopants having breakdown voltages in the range from 20 to 40V/mm and a nonlinearity coefficient  $\alpha$  above 20. The development was based on the discovery that the rapid decomposition of pre-reacted phases from the Bi<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> system into the TiO<sub>2</sub>-rich Bi<sub>2</sub>O<sub>3</sub> liquid phase enhances formation of inversion boundaries in the ZnO grains, which results in the homogeneous grain growth and the microstructure development.

The influence of the organic vehicle and the amount of added varistor powder filler on the rheological characteristics of the pastes and their screen-printing performance was studied. A paste with a high solids load of 70% and good printing characteristics was developed and enables the preparation of dense layers of varistor ceramics with good electrical characteristics at a low sintering temperature of 900 °C, typical for the screen-printing hybrid circuit technology.



**Figure 2:** TEM study of rutile precipitates in chrysoberyl crystals from Pratinhas. (a) Two rutile orientations are observed (R1 and R2). (b) L-shaped cluster of two impinging rutile precipitates enclosing an angle of 98.7°. (c) Isolated rutile precipitate. (d) Structural analysis of chrysoberyl-rutile (Ch|R1) interface. Crystallographic axes of chrysoberyl and rutile are used to determine the orientation relationship  $[001]_{Ch} \parallel [010]_{R(103)}$ . Real space  $4 \times 4$  unit-cells are outlined in yellow. (e) Fast Fourier transform of HRTEM image from Fig. 8b displaying additional reflections from rutile R1 and R2 precipitates (arrows). (f) Reconstructed EDP of chrysoberyl and rutile precipitates calculated with lattice parameters of deformed rutile from the HRTEM analysis (Fig. 8d), with  $(120)_{Ch} \parallel (103)_{R1}$  and  $(120)_{Ch} \parallel (103)_{R2}$ . Reciprocal  $2 \times 2$  unit-cells are outlined (chrysoberyl - grey, R1 - red, R2 - blue).



**Figure 3:** (a) The MFM image of an individual Co-Pt nanowire. (b) Schematic picture of possible magnetization modulation in the nanowire. (c) Saturation magnetization state of an individual Co-Pt nanowire at applied field of  $H_{per} \approx 50$  kA/m. (d) Remanent magnetization of an individual Co-Pt nanowire.



Applications involving **transparent conducting films** (TCFs), such as flat-panel displays and touch screens technologies, are dominated by indium-tin-oxide (ITO). The increasing prices of indium make a strong argument for alternative TCFs with competitive characteristics and a lower price. We demonstrate the potential of highly oriented zinc oxide (ZnO) films grown on glass substrates under low-temperature hydrothermal (HT) conditions at 90 °C from aqueous solutions of Zn-nitrate and Na-citrate. The formation of a continuous ZnO seed-layer with the proper thickness, grain size, connectivity and orientation of the seed-grains on the glass is shown to be essential to achieve the conditions for the growth of highly oriented (0001), smooth, transparent and conductive ZnO films according to the spatially confined oriented growth (SCOG) mechanism. The film grown on a homogeneous seed-layer with a grain size of about 20 nm showed an optical transmittance of up to 82% and a relatively low resistivity for the undoped ZnO ceramic of the order of a few 100  $\Omega$  sq<sup>-1</sup>. Such characteristics are explained by a highly oriented crystalline texture and a high coalescence of the ZnO crystals in these films.

In collaboration with the company VARSİ we continued the development of special varistors for the overvoltage protection of renewable energy systems (solar panels and wind-turbine generators). The result is new types of varistors with a high stability under a dc field for operation under harsh climate conditions (temperature, humidity).

In the development of cost-effective and **environment friendly photovoltaic systems** the Cu<sub>2</sub>ZnSnS<sub>4</sub>-type films (CZTS) showed very promising. CZTS is p-type semiconductor with preferred optical band gap at 1.5eV and a high absorption coefficient made of well abundant and hence cheap elements, which are also nontoxic. We studied the

preparation of CZTS films by sol-gel spin coating and annealing in a sulphur-rich atmosphere at 500°C on flexible metal substrates of Al, Ti, Cu and Mo.

We continued our studies of topochemical defects, epitaxies and phase transformations in **natural and synthetic minerals**. We found that small Cu additions stabilize the formation of mackinawite and the sphalerite (Cu, Fe)S modification. In *American Mineralogist* we published a paper on (101) twins in rutile, where we proposed the formation mechanism of twins in rutile by progressive recrystallization after oxyhydroxide precursor; the (101) twin boundaries are stabilized by the presence of Al-hydroxide and the (301) twin boundaries by the presence of Fe-hydroxide. We also continued our investigations of twinning in spinel and taaffeite-type modulated structures in the spinel-chrysoberyl (MgAl<sub>2</sub>O<sub>4</sub>-BaAl<sub>2</sub>O<sub>4</sub>) system. The PhD student Sandra Drev conducted a three-month specialization at the Max Planck Institute in

Stuttgart, where she focused on the ordering of taaffeite-type modulated structures in Be-doped spinel. In cooperation with dr. Goran Dražič from the National Institute of Chemistry we successfully determined the presence of a single atomic layer of beryllium at the (111) twin boundaries in spinel. In addition to being a major analytical challenge, this was crucial for the confirmation of our theory on topochemically induced twinning. We also determined the local atomic structure of the (130) twin and rutile precipitates in chrysoberyl. The initial atomic model of the twin boundary was proposed based on the HRTEM analyses and a detailed Rietveld analysis of the chrysoberyl structure, performed in cooperation with dr. Matjaž Mazaj from the National Institute of Chemistry. The local atomic model was further optimized by density functional theory (DFT) calculations in cooperation with dr. Matej Komelj. The results of this work were described in a paper that received excellent reviews and is accepted for publication in *American Mineralogist*. In the system ilmenite-hematite we continued our studies of topotaxial transformations during the oxidation of ilmenite to rutile and hematite. First we investigated natural oriented rutile/hematite intergrowths from Mwinilunga in Zambia, where we learned of a complex nature of topotaxial reactions. After a detailed analysis of the rutile/hematite interfaces, nano-inclusion of ilmenite in rutile and precipitates of hematite in rutile, we were able to reconstruct the progressive topotaxial reactions that led to the formation of complex rutile/hematite intergrowths. This work is accepted for publication in *Contributions to Mineralogy and Petrology* (IF=3.02), which is to be the first article published in this prestigious journal by Slovenian authors. The mechanism of ilmenite oxidation was further studied by heating single crystals of ilmenite in an atmosphere of air. We found that during the heating of ilmenite, rutile exsolutions follow a different crystallographic law compared to that of the natural specimens. Based on our studies of naturally and synthetically oxidized ilmenite samples we are able to explain topotaxial crystallographic relationships as a function of temperature and oxygen fugacity. In the past year we also started synthesis procedures for the enhanced growth of multiply twinned rutiles in several subsequent generations, which has potential application value in the development of fractal supports for separation processes and catalysis. In 2014 we started a new research area of twinning in cassiterite, which is isostructural with rutile, and has many potential applications in catalysis and sensor technology due to its excellent optical and electrical properties. We started our investigations by studying natural cassiterite twins, where we have indications that their formation is related to the topotaxial recrystallization over some Fe-oxides, probably magnetite. The identified mechanism of twinning will be further verified by the synthesis under controlled laboratory conditions.

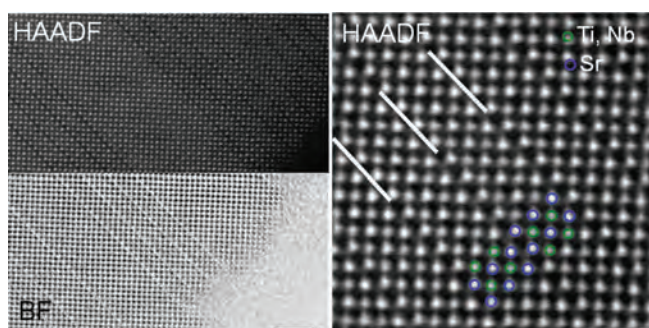


Figure 4: HRSTEM micrograph of RP faults within Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub>, as seen in the [001] zone axis.

In collaboration with research group from Vinča Institute of Nuclear Sciences, Serbia, we studied the relationship between the kinetics of the sorption process and the structure-chemistry properties of  $\text{MgH}_2$  thin films, which are considered to be one of the most promising candidates for the reversible hydrogen storage. To elucidate the rate-limiting step for desorption thin films of  $\text{MgH}_2$  were prepared and irradiated with argon ions. Detailed high-resolution transmission electron microscopy (HRTEM) and selected-area electron diffraction (SAED) studies showed different microstructures between non-irradiated and irradiated films. The non-irradiated thin films are homogeneous, consisting of randomly orientated crystallites. In contrast to the previous case, the irradiated film was signified by large crystal grains imbedded in a crystallites matrix. The SAED analysis showed the coexistence of  $\text{MgH}_2$ ,  $\text{MgO}$  and  $\text{Mg}$  crystal phases.

In collaboration with the research group from Sabanci University, Turkey, we have studied long persistence phosphors, which enable the storage and slow discharge of light. It is anticipated that the incorporation of such a delayed light release source will improve the light-harvesting efficiency for photovoltaic applications. We focused on strontium aluminate (SA) phosphors doped with  $\text{Eu}^{2+}$  and  $\text{Dy}^{3+}$  ions, which are the promising long persistence phosphors candidates for photovoltaics. We showed that the incorporation of boron into the compounds extends the afterglow from minutes to longer than 8 hours. To determine how the electronic structure is modified by the incorporation of boron into the matrix structure we applied electron energy-loss spectroscopy (EELS). Spectral features were interpreted qualitatively as the coordination fingerprints, using reference crystal phases, revealing that the boron is planar 3-fold coordinated, forming  $\text{BO}_3$  units, therefore occupying the interstitial sites in this SA powders.

For the investigations of innovative materials on the micrometre and sub-micrometre scales we have implemented advanced analytical methods: high-resolution scanning electron microscopy (FEGSEM), qualitative and quantitative elemental electron-probe microanalysis (EPMA) with energy-dispersive and wavelength-dispersive X-ray spectroscopies (EDS, WDS) and electron backscatter diffraction (EBSD). These methods were modified and improved, taking into account the specific characteristics of individual materials in order to achieve precise, accurate and reliable analytical results.

Optimized analytical methods were applied for the research of a variety of materials: metallic and ceramic thin films, nanorods, nanoparticles, complex metallic alloys, magnetic materials, perovskite ferroelectrics. Using EBSD we have investigated the microcrystallographic properties of materials, i.e., the crystallinity, crystallographic orientation of phases and texture. In this way we have directly verified the presence of quasicrystals with the so-called “forbidden” 5-fold and 10-fold symmetries, which form in complex alloys, e.g., Al-Mn-Cu-Mg-Si.

We have collaborated with partners from industry and other research institutions performing the analyses and expertise related to the microstructural, quantitative elemental and crystallographic characterization of various materials. The main collaborations were realized with SwatyComet Maribor, Cinkarna Celje, UL-NTF Department of Materials and Metallurgy, University of Ljubljana, RC SIMIT Kidričevo, and the Faculty of Medicine, University of Ljubljana.

One of the important research areas of the department is the implementation of various electron-microscopy analytical techniques within the existing EU project ESTEEM2, such as electron-energy-loss spectroscopy (EELS), high-resolution scanning transmission electron microscopy (STEM, HAADF-STEM), electron holography and the mechanical preparation of the TEM samples. The implementation of various electron microscopy analytical techniques and the possibility for the researchers to access research infrastructure for electron microscopy within the Centre for Electron Microscopy and Microanalysis (CEMM) is of utmost importance for the research.

The researchers at our department are also strongly involved in the promotion of science. One of the activities is a series of scientific lectures for the general public within the action “Science on the street, knowledge and ideas on the go”.

## Organization of conferences, congresses and meetings

1. AdSTEM 2014, European Workshop on Quantitative STEM Imaging, EELS and EDXS, Piran, Slovenia, 29 September–3 October 2014
2. 22nd International Conference on Materials and Technologies, Portorož, Slovenia (co-organizers), 20–22 October 2014
3. REPM2014, Rare Earth and Future Permanent Magnets and Their Applications Workshop 2014, Annapolis, USA, 15–23 August 2014 (members of the International Advisory Board)

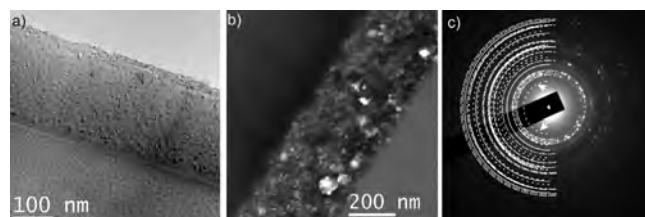


Figure 5: TEM image of a) non-irradiated film and of the b) irradiated film. c) SAED pattern acquired from the irradiated film shows the presence of  $\text{MgH}_2$  (short dashed line),  $\text{MgO}$  (full line) and  $\text{Mg}$  (long dashed line) crystal phases.



- EMAS 2014, 14th European Workshop on Modern Developments and Applications in Microbeam Analysis, Leoben, Austria, 21–24 September 2014, (members of Management Board of the European Microbeam Analysis Society)

## Awards and appointments

- Martina Lorenzetti**, Thomas Luxbacher, Spomenka Kobe, Saša Novak: »Zeta Potential: A Useful Tool to Interpret the Hydrothermally Treated Titanium Behaviour as Biomaterial«, Best oral presentation at the ESB2014 (European Society of Biomaterials) Conference, Liverpool, United Kingdom, 3 September 2014
- Ana Gantar**, Rok Kocen, Saša Novak: »Nanoparticulate bioactive glass-reinforced gellan-gum hydrogels for bone tissue engineering«, Best oral presentation at the 22nd Conference on Materials and Technology, Portorož, Slovenia, 20–22 October 2014

## Patent granted

- Kristina Žužek Rožman, Paul McGuiness, Marko Soderžnik, Dejan Mir, Passive magnetic cradle with THWE mechanism of stopping and positioning, SI24202 (A), Urad RS za intelektualno lastnino, 30.4.2014.

## INTERNATIONAL PROJECTS

- 7FP - ROMEO, Replacement and Original Magnet Engineering Options  
Prof. Spomenka Kobe  
European Commission
- Selective Laser Melting (SLM) and Spark Plasma Sintering (SPS) of Cost Effective Rare-earth based Permanent Magnets for Electrical Machines  
Prof. Spomenka Kobe  
ABB Switzerland Ltd
- 7FP - BioTiNet; Academic-Industrial Initial Training network on Innovative Biocompatible Titanium-based Structures for Orthopaedics  
Prof. Spomenka Kobe  
European Commission
- 7FP - Fusion Expo; Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN-FUSEX  
Prof. Saša Novak Krmpotič  
Ministry of Education, Science and Sport
- 7FP - NANOPYME; Nanocrystalline Permanent Magnets Based on Hybrid Metal-Ferrites  
Asst. Prof. Kristina Žužek Rožman  
European Commission
- 7FP - ESTEEM 2; Enabling Science and Technology through European Electron Microscopy  
Prof. Miran Čeh  
European Commission
- 7FP - MAG-DRIVE; New Permanent Magnets for Electric-Vehicle Drive Application  
Asst. Prof. Matej Andrej Komelj  
European Commission
- 7FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability  
Prof. Saša Novak Krmpotič  
European Commission
- Materials-PPPT-FU, EUROFUSION: WC and SiC Reinforced Tungsten  
Prof. Saša Novak Krmpotič  
European Commission
- Enabling Research-1-FU, EUROFUSION: Advanced SiC/SiC Toward Implementation in Fusion Power Plants  
Dr. Aljaž Iveković  
European Commission
- MODEF - Creazione e Sperimentazione Congiunta di Modelli per l'Ottimizzazione dell'Utilizzo di Energia Fotovoltaica  
Dr. Zoran Samardžija  
Unindustria Rovigo
- COST MP1005, NAMABIO; From Nano to Macro Biomaterials (Design, Processing, Characterization, Modelling) and Applications to Stem Cells Regenerative Orthopaedic and Dental Medicine  
Prof. Saša Novak Krmpotič  
COST Office
- COST ES1205; The Transfer of Engineered Nanomaterials from Wastewater Treatment & Stormwater to Rivers  
Prof. Saša Novak Krmpotič  
COST Office
- CALGAD-X: New Calcium-Gadolinium-X Complex Metallic Alloys

- Prof. Spomenka Kobe  
Slovenian Research Agency
- Study of Chemical Strain in Perovskites Doped With Aliovalent Cations by Applying In-Situ X-Ray Diffraction, Dilatometry and Advanced Transmission Electron Microscopy Techniques  
Asst. Prof. Sašo Šturm  
Slovenian Research Agency
  - Biomimetic Characterisation of Bioactive Composit Scaffolds for Bone and Osteochondral Tissue Repair  
Prof. Saša Novak Krmpotič  
Slovenian Research Agency
  - Development of Oxide Thermoelectric Materials for Waste-heat Recovery into Electricity  
Asst. Prof. Slavko Bernik  
Slovenian Research Agency
  - Characterisation of Growth Features and Planar Defects in Crystals Grown Under Hydrothermal Conditions  
Asst. Prof. Nina Daneu  
Slovenian Research Agency
  - Advanced Methods and Technologies for Processing of a New Generation of ZnO-based Varistor Ceramics  
Asst. Prof. Slavko Bernik  
SICCAS, Shanghai, China
  - NSFM: Novel Smart Filtration Media  
Asst. Prof. Kristina Žužek Rožman
  - Services for the Exports  
Dr. Zoran Samardžija

## RESEARCH PROGRAM

- Nanostructured Materials  
Prof. Spomenka Kobe

## R & D GRANTS AND CONTRACTS

- Twinning, Epitaxy and Phase Transformations in Minerals  
Asst. Prof. Nina Daneu
- Atomic-scale Studies of Initial Stages of 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  
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 Dražič
- Novel Functionalized Nanomaterials for Applications as Nano- or Biosensors/Actuators/Bioresponsive (Carrier) Systems  
Asst. Prof. Kristina Žužek Rožman

7. Structure and Chemical Composition Study of Surfaces and Interfaces with High Resolution Scanning Transmission Electron Microscopy at Atomic Level  
Asst. Prof. Aleksander Rečnik
8. Bio-responsive Magneto-optically Coupled Nanomaterial-based Systems for Innovative Skin Cancer Treatments  
Asst. Prof. Sašo Šturm
9. Microbial Adhesion Management on Material Surfaces  
Asst. Prof. Goran Dražič
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 McGuinness
12. Materials and Technologies for Applications of ZnO-based Thick-film Varistors and Oxide Thermoelectrics  
Asst. Prof. Slavko Bernik
13. Colour, Absorption and Protective Nanolayer Coatings for Aluminium Alloy  
Prof. Miran Ceh
14. Innovative Production Systems for Vaccines and Regenerative Medicine  
Asst. Prof. Aleksander Rečnik
15. Development of the Model of the System for Intelligent Support of the Selection of Suitable Powder Material when Developing Sintered Products  
Prof. Saša Novak Krmpotič
16. Modification of TiO<sub>2</sub> Nanoparticle Surface: Prevention of Agglomeration and

- Preservation of Intrinsic Properties  
Asst. Prof. Aleksander Rečnik
17. Tridimensional Bioactive Glass and Biopolymer Composite Scaffolds for Treatment of Osteochondral Defects Developed due to the Articular Cartilage Lesions  
Dr. Nataša Drnovšek
  18. Irradiation and Analysis of Si Samples  
Prof. Saša Novak Krmpotič
  19. From the Synthesis of Metal Oxides to the Humidity and Oxygen Prototype Nanosensors  
Dr. Kristina Žagar

## NEW CONTRACTS

1. The Study of Self-cleaning and Abrasion Resisting Properties of Carbon-, Para-aramid- or Glass-fibre-based Composite Materials by Applying Photocatalytic and/or Mechanical Resistant Nanoparticles  
Asst. Prof. Sašo Šturm  
CDT Group, d. o. o.
2. Multipole Magnetisation of NdFeB Bonded Magnets for Rotor Application  
Prof. Spomenka Kobe  
Kolektor KFH, d. o. o.
3. Cooperation within the R&D Program of the Company Akripol  
Prof. Saša Novak Krmpotič  
Akripol d. o. o.

## VISITORS FROM ABROAD

1. Yibo Zhou, Shanghai Institute of Ceramics, Chinese Academy of Science - SICCAS, Shanghai, China, 16 January–11 July 2014
2. Francesco Gucci, Università di Torino, Turin, Italy, 4 March–31 May 2014
3. Prof. Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 17–22 January 2014, 30 March–4 April 2014, 3–4 June 2014, 17–19 July 2014, 27 August–3 September 2014
4. Prof. Michael Zehetbauer, Fakultät für Physik, Universität Wien, Vienna, Austria, 24 April 2014
5. Federica Pirani, Università di Torino, Turin, Italy, 2 April–30 June 2014
6. Luisa Belardi, Università di Torino, Turin, Italy, 2 April–30 June 2014
7. Prof. Michael Gasik, Aalto University Foundation, Aalto, Finland, 3–4 April 2014
8. Prof. Ikka Kangasniemi, ID Creations oy, Turku, Finland, 3–4 April 2014
9. Idris Sorar, Mustafa Kemal University, Department of Physics, Antalya/Hatay, Turkey, 19 May 2014
10. Dr. Thomas Luxbacher, Anton Paar, Graz, Austria, 3 June 2014
11. Prof. Kazuki Nakanishi, Department of Chemistry, Kyoto University, Kyoto, Japan, 4 June 2014
12. Stephen Kyle-Henney, TISICS Limited, Hampshire, United Kingdom, 16–17 June 2014
13. Prof. Frans Kools, Technische Universiteit Eindhoven, Eindhoven, The Netherlands, 26 June 2014
14. Dr. Richard Wheeler, Edinburgh Scientific, Edinburgh, United Kingdom, 11 August 2014
15. Michele Carenini, Edinburgh Scientific, Edinburgh, United Kingdom, 11 August 2014
16. Prof. Mehmet Ali Gulgun, Prof. Cleva Ow Yang, Meltem Asilturk in Yener Kuru, Sabanci University, Istanbul, Turkey, 29 September–8 October 2014
17. Samed Çetinkaya, Technology and R&D Application and Research Center, Mustafa Kemal University, Hatay, Turkey, 7–15 October 2014
18. Dr. Heike Schlörb, Institut für Metallische Werkstoffe – IMW, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden - IFW Dresden, Germany, 22–27 October 2014
19. Dr. Milivoj Plodinec, Institut Rudjer Bošković, Zagreb, Croatia, 17–22 November 2014
20. Dr. Andreja Gajović, Institut Rudjer Bošković, Zagreb, Croatia, 22–28 December 2014
21. Koichi Sakuta, Technology Research Association of Magnetic Materials for High-Efficiency Motors - MagHEM, Tokyo, Japan, 18 November 2014
22. Hirokazu Kubo, Intermetallics Co. Ltd., Kyoto, Japan, 18 November 2014
23. Hiroyuki Kobayashi, T&T Innovations Inc., Otake, Japan, 18 November 2014
24. Noritsugu Sakuma, Toyota Motor Corporation, Shizuoka, Japan, 18 November 2014
25. Sho Goto, Denso Corporation, Kariya, Aichi, Japan, 18 November 2014
26. Shintaro Arakai, Daikin Industries Ltd., Osaka, Japan, 18 November 2014
27. Masaki Yasuoka, AIST, Nagoya, Japan, 18 November 2014
28. Kaoru Iizuka, Nedo, Japan, 18 November 2014
29. Dr. Laszlo Peter, Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, Hungary, 27–28 November 2014
30. Prof. Mariana Calin, Institut für Komplexe Materialien, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden - IFW, Dresden, Germany, 18–20 December 2014

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  16. Dr. Petra Jenuš
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  19. Dr. Matejka Podlogar
  20. Dr. Marko Soderžnik
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  27. Rok Kocen, B. Sc.
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  31. *Dr. Alenka Lenart, left 18. 08. 14*
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  41. Špela Klemenčič, B. Sc.
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42. Martin Topole

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

- Muhammad Shahid Arshad, Darja Pečko, Sašo Šturm, Juan Escrig, Matej Komelj, Paul J. McGuinness, Spomenka Kobe, Kristina Žužek Rožman, "Angular dependence of the coercivity in electrodeposited Co-Pt nanostructures with a tube-wire morphology", In: Proceedings of the INTERMAG 2014, IEEE International Magnetism Conference, May 4-8, 2014, Dresden, Germany, *IEEE trans. magn.*, vol. 50, no. 11, pp. 2302904-1-2302904-4, 2014.
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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 various advanced materials, especially magnetic materials, semiconducting oxides, and optical materials. Special attention is given to nanostructured materials, such as ferrofluids, functionalized nanoparticles for use in biomedicine, multifunctional nanocomposites, magnetic coatings, and fluorescent materials.***

In 2014 our investigations have focused on several important materials, i.e., materials containing magnetic nanoparticles, multifunctional nanocomposites, fluorescent materials, and semiconducting materials for the preparation of thermistors.

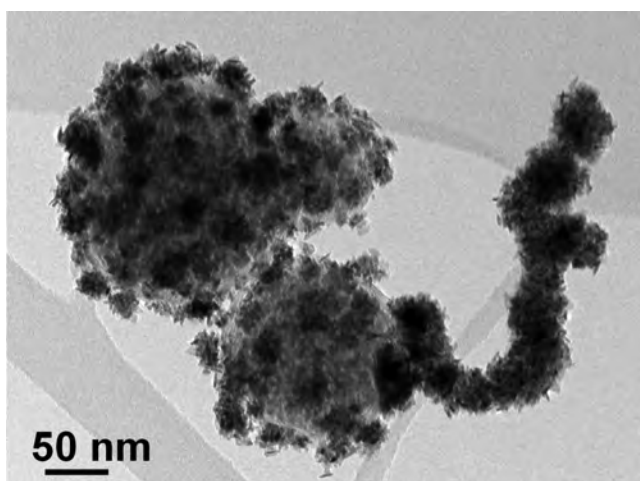
The research of nanoparticles-based materials is continuously focused on engineering nanoparticles' surface properties. The engineering of surface properties is of key importance for nanoparticle applications, as well as for their assembly into composite materials. The surface properties are usually engineered by bonding different functionalization molecules onto the nanoparticles' surfaces. The functionalization molecules provide specific functional groups for the further (bio)conjugation of different molecules needed for a specific application. The layer of organic molecules also defines the electric charge at the surfaces and the interactions between the nanoparticles in a liquid medium. It also significantly determines the interactions of the nanoparticles with biological systems. A part of the research in 2014 was devoted to the engineering of surface properties of superparamagnetic iron-oxide maghemite nanoparticles using the adsorption of different amino acids onto their surfaces. The application of different amino acids in the engineering of nanoparticles' surface properties and their functionalization is broadly discussed in the scientific literature. In theory, a large number of amino acids enable changing of the surface properties across a broad range. However, the literature results are inconsistent. To explain the discrepancies between our results and some findings from the literature, we cooperated with researchers from the Faculty of Chemistry and Chemical Technology, University of Ljubljana, on systematic research of aspartic acid adsorption onto maghemite nanoparticles, especially when the nanoparticles are synthesized by coprecipitation in the presence of the amino acid. The results show that the amino acids are adsorbed onto the nanoparticles' surfaces in the form of large associates. The formation of molecular associates has a major influence on the colloidal properties of the suspensions and their potential applications.

A large part of the research was devoted to the controlled assembly of superparamagnetic iron-oxide nanoparticles into nanoclusters, which can be applied as magnetic carriers in different applications related to magnetic separation. The magnetic separation is based on the selective bonding of targeted species, i.e., ions, molecules, cells, or microorganisms, onto the magnetic carriers followed with their separation from the mixture using an external magnetic field. The magnetic carriers have to be composed of magnetic nanoparticles that are small enough to be in the superparamagnetic state, i.e., below approximately 15 nm. Individual superparamagnetic nanoparticles are usually not efficient in magnetic separation, because of the too small magnetic force acting on them in a magnetic-field gradient, which is the result of their very small volume. For an improved ability of magnetic separation, the superparamagnetic nanoparticles have to be assembled into nanoclusters, optimally with a size from 50 to 100 nm. The superparamagnetic nanoclusters were self-assembled from superparamagnetic iron-oxide maghemite nanoparticles in the suspensions. The nanoclusters' surfaces were coated with a thin silica shell, which enabled the effective covalent bonding of different functionalization molecules onto their surfaces. The fluorescent molecules were incorporated into the silica shell for the tracking of the nanoclusters with methods based on fluorescence microscopy. In cooperation with researchers from the Vinča Institute, Serbia, the magnetic



Head:  
**Prof. Darko Makovec**

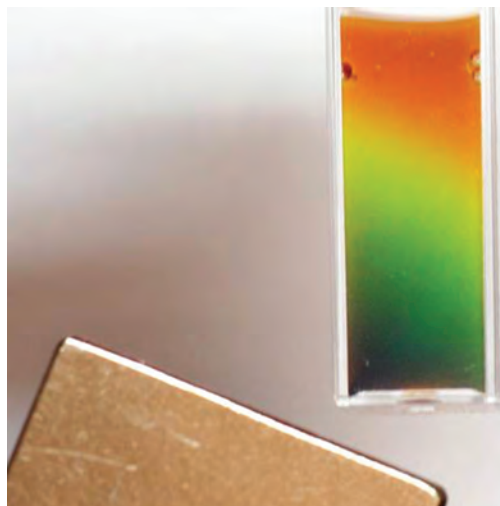
**Applications of superparamagnetic nanoclusters in magnetic separation and in magneto-optic suspensions were studied.**



*Figure 1: Superparamagnetic nanoclusters coated with catalytic ruthenium nanoparticles.*

properties of the superparamagnetic nanoparticles were systematically studied with special attention paid to inter-particle interactions inside the nanoclusters.

An important part of the research in 2014 has been devoted to the testing of superparamagnetic nanoclusters in applications that are based on magnetic separation. In such applications the commercially available superparamagnetic nanoclusters produced by Nanos Sci. (<http://nanos-sci.com/>), a spin-out company of the JSI, are normally used. Typical example of such applications is the use of superparamagnetic nanoclusters for the immobilization of (bio)catalysts, which enables their magnetic separation from the medium after catalytic reactions. Different strategies of bio-conjugation of chloroperoxidase and aldolase enzymes onto the functionalized nanoclusters were studied in cooperation with researchers from Universidad Autònoma de Barcelona, Spain, to prepare magnetically-separable nano-biocatalysts. Nano-biocatalysts were tested in multi-enzymatic synthesis procedures for the stereo-selective synthesis of aminopolyols and iminocyclitols, which are important in pharmacy and nutraceuticals.



*Figure 2: The inner periodic structure with the periodicity corresponding to a wavelength of visible light is established in a suspension of superparamagnetic nanoclusters under the influence of a magnetic field, when the suspension is exposed to a permanent magnet. The periodicity depends on the magnetic-field strength, and as the result, the colour of the light diffracted by the suspension.*

The superparamagnetic nanoclusters can also be used as a support for metallic catalysts. Metallic ruthenium was deposited onto the surfaces of the superparamagnetic nanoclusters by the heterogeneous nucleation of ruthenium during the reduction of ruthenium acetylacetonate in the suspension of nanoclusters in 2-propanol (Figure 1). The catalytic material is tested in collaboration with researchers from the National Institute of Chemistry. The catalyst is being tested for the catalysis of transfer hydrogenation of levulinic acid in 2-propanol and the hydrogenation of levulinic acid using molecular hydrogen.

Besides magnetic separation, the magnetic nanoclusters could also be interesting in many other applications where a relatively large force acting on the nanocluster in a magnetic field gradient could be beneficially exploited.

Magnetic drug delivery and cell-transfection (magnetofection) using magnetic nanoclusters are the most promising applications in the biomedical field. In collaboration with researchers from the Faculty of Pharmacy, University of Ljubljana, we have developed various magnetic nanostructured materials that may show significant advantages compared to the known delivery systems.

In collaboration with researchers from the Department of Condensed Matter, JSI, we have performed research on exploiting the possibilities of using of superparamagnetic nanocluster suspensions in photonics. Interesting optical properties in a visible spectrum have been observed as a consequence of the nanocluster ordering into periodic structures under the influence of a magnetic field. The optical absorption/diffraction properties of the suspensions can already be manipulated by applying relatively weak changes in the magnetic field (Figure 2).

In collaboration with the Nanos Sci. Company we have performed the R&D of new magnetic nanostructures, which are based on a magnetic assembly of superparamagnetic nanoclusters in suspensions into higher nano-architectures, such as permanent one-dimensional (1D) nanochains and two-dimensional (2D) nanoribbons (Figure 3). These nanostructures show radically new and very promising possibilities in medicine and technology, for example, in magneto-rheology.

In order to exploit the advantages of the anisotropic magnetic nanostructures, we studied the magneto-rheological effect in their suspensions. When a suspension of such nanostructures is exposed to a magnetic field, its rheological properties quickly change. We have established a research collaboration in the field of magneto-rheology with the world-leading group from the Technical University Dresden, Germany. In the scope of this collaboration

we have prepared suspensions of specially adjusted magnetic nanostructures dispersed in various carrier liquids.

In collaboration with researchers from the Department of Condensed Matter, JSI, we have also researched the magnetic assembly of the nanochains into various phases that are promising in nano-optics. Our preliminary results showed that highly magnetically responsive nanochains can form

the desired liquid-crystal phase when exposed to relatively weak magnetic fields.

A part of our research was devoted to the detailed characterisation of composite nanoparticles synthesized using a coating of thin shells of magnetic iron oxide onto different core nanoparticles with a simple precipitation from aqueous solutions. By coating a shell of soft-magnetic spinel iron oxide maghemite ( $\gamma\text{-Fe}_2\text{O}_3$ ) onto hard-magnetic barium-hexaferrite ( $\text{BaFe}_{12}\text{O}_{19}$ ) platelet cores the "sandwich"-type composite nanoparticles were synthesized. The spinel layers grow epitaxially on the hexaferrite core. A direct contact between the two magnetic phases results

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**Magnetic assembly of superparamagnetic nanoclusters in highly anisotropic nanostructures: one-dimensional chain-like nanorods and two-dimensional nano-belts.**

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in magnetic coupling and, consequently, in a large increase in the energy product  $|BH|_{\max}$  by more than twice compared to the  $|BH|_{\max}$  of the core nanoparticles. In 2014 the main focus was on the synthesis of the composite nanoparticles by coating a maghemite layer onto hexaferrite cores with strong magnetic properties. Such core nanoparticles can be synthesized using special dopants, such as Sc. However, with the improved hard-magnetic properties the agglomeration of nanoparticles due to magnetic dipole-dipole interactions becomes critical during the synthesis of the composite nanoparticles. It is necessary to improve colloidal properties of the core-nanoparticles suspensions using surfactants. The use of the surfactants increases the complexity of the coating process, since they usually enter the reactions. We succeeded in preparing a stable aqueous suspension of hard-magnetic-core nanoparticles, which enabled the synthesis of sandwich-type nanoparticles, approximately 70 nm wide and 7 nm thick, which showed greatly improved properties. The colloidal properties of their aqueous suspensions were systematically studied, as the preparation of stable colloids is a prerequisite for their further testing in biomedical applications. A part of the research was also devoted to the possibility of coating shells made of other magnetic spinels, especially of hard-magnetic cobalt ferrite, onto the different core nanoparticles.

We continued the research devoted to magnetic nanoparticles with an adaptable Curie temperature ( $T_c$ ) for use in self-regulating magnetic hyperthermia. The  $T_c$  limits the temperature to which the nanoparticles are being heated in an external magnetic field, and thus an external temperature control is not required. In cooperation with the Faculty of Chemistry and Chemical Technology, University of Maribor, we have studied the synthesis and properties of nanoparticles made of those magnetic materials, where the  $T_c$  can be tuned to the therapeutic values by adapting their composition. The main focus was on spinel ferrite Mg(Ti)  $Fe_2O_4$  and on different alloys from the systems Cu-Ni and Cr-Ni.

We also cooperated in nanotoxicology research with the Biotechnical Faculty, University of Ljubljana, where we provided our expertise in the synthesis, functionalization and characterization of nanoparticles.

The research was also devoted to the synthesis of magnetoelectrics - composites in which magnetic and ferroelectric properties are mechanically coupled. The properties of such composites depend on the basic properties of constituent phases and on the specific phase distribution in the material. The anisotropic  $CoFe_2O_4$  3D structures can be used as a basis for magnetoelectric composites with the 1-3-type structure. We studied their preparation using the electrophoretic deposition of  $Pb(Zr,Ti)O_3$  on top of  $CoFe_2O_4$  columns in cooperation with the Electronic Ceramics Department, JSI. In this kind of composites it is necessary to prevent current leakage through the sample thickness via the  $CoFe_2O_4$  columns. Therefore, the height of the  $CoFe_2O_4$  columns was adjusted in such a way that the  $Pb(Zr,Ti)O_3$  deposit was thick enough to completely cover the  $CoFe_2O_4$  columns. An additional problem that is still being studied is related to the co-sintering of the two materials. In previous research we determined the optimum co-sintering parameters for similar bulk ceramic composites, which included pre-firing of the  $CoFe_2O_4$  at 700 °C followed by a co-sintering at 950 °C. However, additional stress induced during the sintering on a substrate resulted in crack formation in the film composite layers of the 1-3 type.

A part of research has been devoted to the deposition of thick films from nanoparticle suspensions. A comparative study of the assembly of ferrimagnetic  $CoFe_2O_4$  in  $BaFe_{12}O_{19}$  nanoparticles in a magnetic field elucidated the effect of magnetocrystalline structure and particle shape on the morphology and crystallographic and magnetic alignment of the deposits. While the symmetric  $CoFe_2O_4$  nanoparticles assemble in a magnetic field into columnar structures, the  $BaFe_{12}O_{19}$  nanoplates align with the substrate (Figure 4). Such an alignment of nanoplates is a consequence of the coinciding magnetic and crystallographic alignment and enables the preparation of magnetically anisotropic films. An inferior magnetic anisotropy of the  $CoFe_2O_4$  columns results from a different preferential orientation of the nanoparticles in comparison to their magnetic easy axis.

The studies of hexaferrite materials were focused on the incorporation of  $BaFe_{12}O_{19}$  nanoplates into various matrices, like liquid crystals (in cooperation with the Department of Condensed Matter, JSI) and polymers (in cooperation with Faculty of Chemistry and Chemical Technology, University of Maribor). For this purpose we developed various stable suspensions of  $BaFe_{12}O_{19}$  nanoplates doped with  $Sc^{3+}$  in alcohols (from propanol to hexanol). The composite preparation is significantly affected by the evaporation rate of the suspension solvent and its compatibility with other reagents. Relatively highly concentrated suspensions (15 g/l nanoplates) can be obtained in t-butanol. For the preparation of the suspensions of  $BaFe_{12}O_{19}$  nanoplates in nonpolar and weakly polar liquids dodecylbenzenesulfonic acid, used during the nanoparticles synthesis, was replaced by a ricinoleic acid. This enabled the preparation of stable suspensions in hexane, toluene and methylmethacrylate for the subsequent development

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**We showed that concentrated suspensions of ferrimagnetic  $BaFe_{12}O_{19}$  nanoplatelets can be obtained and used for the preparation of liquid-crystal and polymer composites with multiferroic and magneto-optic behaviour.**

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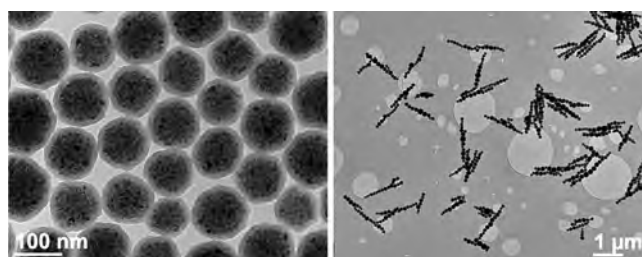


Figure 3: Superparamagnetic nanoclusters and magnetically assembled chain-like nanorods.



of composites containing a high concentration of  $\text{BaFe}_{12}\text{O}_{19}$  nanoplates. This is crucial for a material with applicable magnetic, multiferroic and magneto-optic properties. A significant magneto-optic response was shown in the liquid-crystal and polymer nanocomposites.

We have intensified research devoted to fluorescent optical materials. Fluorescent nanoparticles can be applied in various optical elements and are also proposed as alternative bio-markers in imaging diagnostic techniques for

**We pointed out the problematics for the application of fluorescent fluoride nanoparticles in biomedicine due to their partial dissolution in water.**

medicine. We studied the synthesis of fluoride nanoparticles doped with lanthanides. The main focus was towards the control of the particle size, suspension stability and chemical stability of fluorides in an aqueous environment. Namely, the nanoparticles for bio-medicine should be chemically and colloiddally stable in aqueous media. We showed that fluoride nanoparticles with different compositions (binary and ternary) partly dissolve in water,

which limits their applicability in biomedicine. The dissolution studies were conducted in cooperation with the Department for Inorganic Synthesis and Technology, JSI. The dissolution degree depends strongly on the pH and thermodynamic stability of the nanoparticle's crystal structure. For example, the dissolution degree of  $\text{NaYF}_4$  nanoparticles with a metastable cubic structure was significantly higher than that of the nanoparticles of the same composition, but with a thermodynamically stable hexagonal structure. The thermodynamic stability also coincides with the fluorescence efficiency, which was studied in cooperation with the Department for Complex Matter, JSI. Silica coating was first tested for the protection of fluoride nanoparticles in water but the results were not promising. Currently, we are developing an amphiphilic protective coating based on co-polymers.

A part of the research on fluorescent materials was devoted to the incorporation of fluorescent nanoparticles in optical fibres. For this purpose the size of the fluorescent nanoparticles should be controlled and compatible

with the relevant technology. These studies are conducted in the frame of a common project with a company Optacore. During the last year we focused on the synthesis of binary fluorides, which show superior thermal and chemical stability at high temperatures and in a  $\text{SiO}_2$  matrix, in comparison to, otherwise preferred, ternary fluorides, which is of crucial importance in the optical-fibre technology.

The basic research of semiconducting ceramics was devoted to the origin of the PTCR effect in  $\text{BaTiO}_3$  ceramics. We have shown that it is possible to prepare the PTC thermistors on the basis of  $\text{BaTiO}_3$  ceramics without donor doping when a composite of conductive and non-conductive phases is formed. Due to dimensional changes in the  $\text{BaTiO}_3$  ceramics at the Curie

temperature there is an interruption of connections in the conductive phase that leads to the PTCR anomaly.

In the field of high-temperature thermistors (PTC resistors) we have investigated the possible procedures for the preparation of ferroelectric ceramics in the system  $\text{BaTiO}_3\text{-Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ . The PTC resistors displaying Curie temperature of 180 °C and low room-temperature specific resistivity were developed. Unlike the high-temperature PTC resistors available in the market the developed material contains no toxic lead.

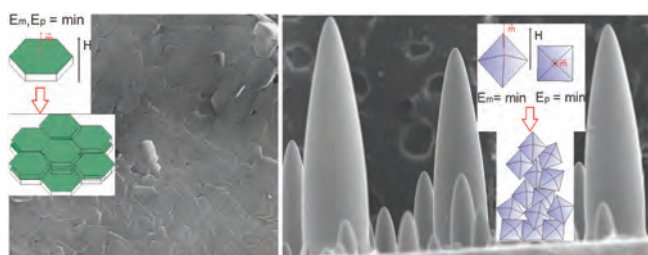


Figure 4: The effect of a magnetocrystalline structure and shape of ferrimagnetic nanoparticles on their assembly in a magnetic field.

### Some outstanding publications in the past year

1. Lisjak, D., Jenuš, P., Mertelj, A.: The influence of the morphology of ferrite nanoparticles on the directed assembly into magnetically anisotropic hierarchical structures. *Langmuir*, 2014, 30, 6588-6595
2. Jenuš, P., Lisjak, D., Kuščer, D., Makovec, D., Drogenik, M.: The low-temperature cosintering of cobalt ferrite and lead zirconate titanate ceramic composites. *Journal of the American Ceramic Society*, 2014, 97, 74-80
3. Kralj, S., Makovec, D.: The chemically directed assembly of nanoparticle clusters from superparamagnetic iron-oxide nanoparticles. *RSC advances*, 2014, 4, 25, 13167-13171 K8

### Awards and appointments

1. Peter Dušak: Best paper according to active participants, Ljubljana, Jožef Stefan International Postgraduate School's Student Council, Preparation of Magnetically-Modified *Oenococcus Oeni*

## INTERNATIONAL PROJECTS

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. COST IC1208; Integrating Devices and Materials: A Challenge for New Instrumentation in ICT<br/>Prof. Darko Makovec<br/>COST Office</li> </ol> | <ol style="list-style-type: none"> <li>2. Superparamagnetic Iron-oxide Nanoparticles and Nanoclusters: Synthesis, Interparticle and Inter-cluster Interactions, Magnetic Moment and Practical Applications<br/>Prof. Darko Makovec<br/>Slovenian Research Agency</li> </ol> |
|---|---|

## RESEARCH PROGRAM

1. Advanced Inorganic Magnetic and Semiconducting Materials  
Prof. Darko Makovec

## NEW CONTRACTS

1. Optical Fibers doped with Fluorescent Nanoparticles  
Asst. Prof. Darja Lisjak  
Optacore, d. o. o.

2. Research and Development of PTCR-effect Semiconducting Ceramics without Environmentally Harmful Lead Oxide  
Dr. Igor Zajc  
Stelem, d. o. o., Žužemberk
3. Characterization of the Reference and Synthesis of Iron-oxide Nanoparticles' Suspension  
Prof. Darko Makovec  
Lek, d. d.
4. Development of Synthesis of Iron-oxide Core similar to the Reference  
Prof. Darko Makovec  
Lek, d. d.

## VISITORS FROM ABROAD

1. Gerard Masdeu, Universitat Autònoma de Barcelona, Barcelona, Spain, 1 May–31 July 2014
2. Dr. Federico Cebollada, Universidad Politécnica de Madrid, Madrid, Spain, 2–5 April 2014
3. Ulla Kanerva, VTT Technical Research Centre of Finland, Tampere, Finland, 29 May–31 August 2014

## STAFF

### Researchers

1. Dr. Sašo Gyergyek
2. Asst. Prof. Darja Lisjak
3. Prof. Darko Makovec, Head
4. Dr. Igor Zajc

### Postdoctoral associate

5. Dr. Slavko Kralj

### Postgraduates

6. Blaž Belec, B. Sc.

7. Peter Dušak, B. Sc.
8. Helena Macut, B. Sc.
9. Olivija Plohl, B. Sc.
10. Klementina Pušnik, B. Sc.  
Technical and administrative staff
11. Bernarda Anželak, B. Sc.

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2. Blaž Belec, Darko Makovec, "Synthesis of composite nanoparticles using coating of the core nanoparticles with cobalt ferrite layers", In: *Zbornik: 1. del: part 1*, 6. študentska konferenca Mednarodne podiplomske šole Jožefa Stefan = 6th Jožef Stefan International

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## MENTORING

1. Petra Jenuš, *Assembly of magnetic nanoparticles as a basis for the preparation of hierarchically structured materials*: doctoral dissertation, Ljubljana, 2014 (mentor Darko Makovec; co-mentor Darja Lisjak).
2. Rok Brišar, *Application of magnetized yeast cells in beer fermentation*: master's thesis, Ljubljana, 2014 (mentor Marin Berovič; co-mentor Darko Makovec).

# DEPARTMENT FOR ADVANCED MATERIALS

# K-9

*At the Advanced Materials Department, novel materials are developed by an understanding of the mutual dependence of their structural and functional characteristics. Contemporary technologies, which enable the synthesis of materials with atomic- and microstructural-scale precision, are applied to prepare beforehand-designed structured ceramics, thin films, and nanoparticles with the desired crystal structure, chemical composition, and microstructure. Among our important objectives is the development of: i) new oxide materials for efficient high-temperature thermoelectric energy conversion, ii) new materials with improved antibacterial and photocatalytic effects, and iii) novel functional oxide materials for various electronic applications.*

## Thermoelectric materials

In the scope of the research on oxide materials as possible candidates for p-type thermoelements in high-temperature thermoelectric modules we continued our investigations of coherently intergrown layered cobaltates  $\text{Ca}_{1-x}\text{Na}_x\text{Co}_4\text{O}_9$ , which we found to be promising in terms of environmental and high-temperature stability. Atomically resolved transmission electron microscopy, performed with Cs-probe corrected scanning transmission electron microscopy, revealed a diversity between the octahedral  $\text{CoO}_2$  layers within the individual grains. The prismatic sites between the layers can be occupied by sodium and calcium ions or the interlayer space can be occupied with the three-layer  $\text{CaO-CoO-CaO}$  rock-salt type stacking. Parts of the individual grains exhibit a structural ordering of the interlayer ions in a zig-zag manner, which was confirmed to be the most stable variant by density functional theory (DFT) calculations. Using electron-energy-loss spectroscopy (EELS) we probed individual  $\text{CoO}_2$  layers neighbouring different interlayer structural arrangements and found that the oxidation state of cobalt ions and, consequently, the electrical charge within the octahedral layers is not significantly affected by the apparent interlayer structure. These observations imply that the observed differences in the structure between the octahedral  $\text{CoO}_2$  layers could also be a consequence of an out-of-zone rotation of the interlayer stacking. The spontaneous interlayer diversity in intergrown cobaltates appears promising for the design of new thermoelectric heterostructures.

As an n-type candidate we investigated the donor-doped perovskite  $\text{CaMnO}_3$ , which exhibits temperature-stable electrical properties. By inducing the formation of Ruddlesden-Popper polytypic faults with excess  $\text{CaO}$  we were able to control the microstructural development and transport properties of the ceramics. With the appropriate amount of excess  $\text{CaO}$ , a grid-like morphology was obtained, which resulted in a threefold decrease of the thermal conductivity. Furthermore, with the introduction of planar faults within the perovskite grains, the electrical transport properties change, resulting in a transition from semiconducting to metallic behaviour and an increase in the Seebeck coefficient. These observations suggest that electrically insulating polytypic faults induce a low-dimensional character within the conductive perovskite matrix.

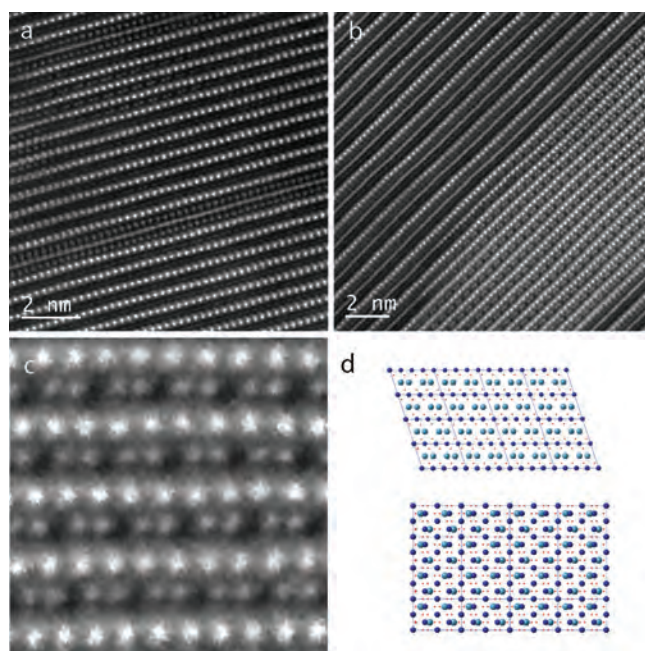
In addition to previous investigations we also focused on the synthesis of novel functional materials based on layered titanium disulfide (Figure 2), with optimized electrical and thermal transport properties. The titanium disulfide forms thermodynamically stable natural superstructures on (self) intercalation and consequently possesses the properties of a highly mobile semiconductor with a low thermal conductivity. Apart from that, it is non-toxic, has a low mass density, and consists of abundant and low-cost elements. Dihalcoenides of this type would be a good replacement for toxic, scarce and expensive materials based on bismuth telluride, which currently have no suitable alternatives as thermoelectric materials in the range of low and medium temperatures. Intercalated  $\text{TiS}_2$  crystals of various morphologies were prepared with solid-state and solvothermal synthesis. In order to pre-



Head:

**Prof. Danilo Suvorov**

**Gallium nanoparticles on hydroxyapatite are a new biomaterial with an antibacterial action.**



*Figure 1. Structural diversity between  $\text{CoO}_2$  layers of intergrown cobaltates: a) rock-salt stacking of  $\text{CaO-CoO-CaO}$ , b) rock-salt stacking and ordering of calcium ions, c) close-up of ordered calcium ions and d) calculated structural model with ordered calcium ions between the  $\text{CoO}_2$  layers viewed along the  $[010]$  and  $[001]$  directions.*



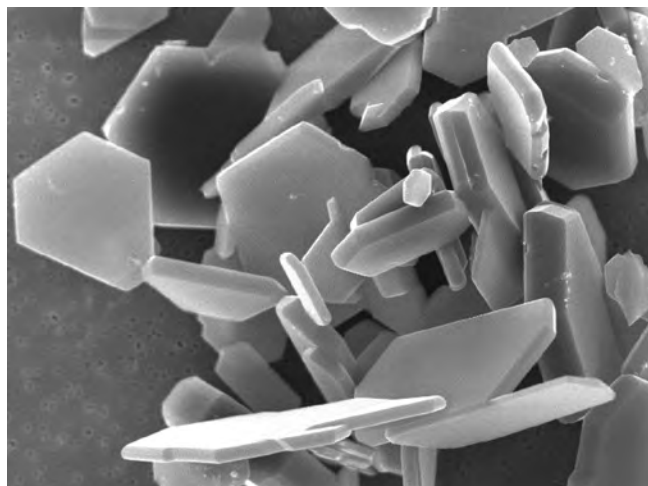


Figure 2. SEM image of layered  $TiS_2$  crystals.

serve the desired structure, as-prepared starting materials were densified to the bulk by PECS (pulsed electric current sintering). It is shown that the structuring could have a significant impact on the electrical and thermal transport properties of these materials.

### Photocatalytic and antibacterial materials

The photocatalytic efficiency of a wide-band-gap semiconductor  $TiO_2$  was enhanced in the ultraviolet range and also shifted to the visible region, by the coupling of  $TiO_2$  anatase nanoparticles with noble-metal (Au) nanoparticles. The  $TiO_2$ /Au nanocomposites were formed using a bifunctional bridging linker that contained both the carboxylic group and the thiol group to enable binding to the  $TiO_2$  and the Au nanoparticle surfaces, respectively. Additionally, the bifunctional bridging linker served as a capping agent for the noble-metal particles, thus preventing their growth and agglomeration. The homogeneously distributed Au particles (4-10 nm) were attached to the  $TiO_2$  particles (~10 nm) to form an effective contact between the two phases. In this way the life-time of the  $TiO_2$  photo-induced charge carriers

was prolonged and the UV photocatalytic activity was enhanced. The plasmonic properties of the Au induced a visible-light response of the material. The prepared composite effectively degrades the organic dye methylene blue and inhibits the growth of the bacteria *Escherichia coli*.

For photocatalytic applications we also synthesized doped (Ce, Zr, Si) anatase with spherical particles ranging from 2 to 7  $\mu m$ . The particles exhibit a mesoporous microstructure and consisted of nanosized primary crystallites with a size up to 20 nm, depending on the synthesis parameters. The obtained doped anatase exhibits interesting photocatalytic properties, even being calcined at 1050 °C.

In 2014 we continued our research on antibacterial materials that include gallium components. We developed new nanocomposite materials that combine bioactive (hydroxyapatite) and antibacterial (metallic nanoparticles) components.

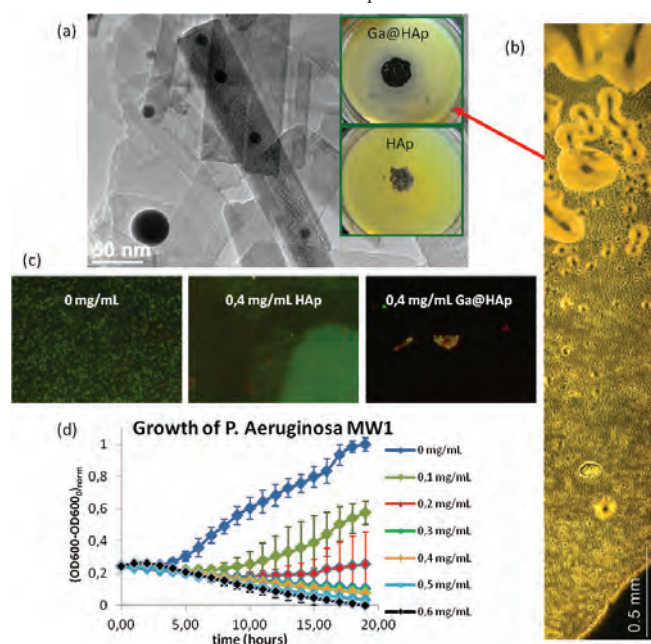


Figure 3. Ga nanoparticles on hydroxyapatite and their antibacterial action against *P. Aeruginosa* MW1: (a) diffusion antibiogram; (b) inhibition zone under phase-contrast microscope with the material at the bottom (black) and the edge of the inhibition zone at the top; (c) merged images of green (live+dead) and red (dead bacteria) fluorescence for *P. Aeruginosa* under fluorescence microscope after incubation without any material, with HAp and with Ga@HAp, respectively; (d) microdilution antibiogram assay of suspension with different concentrations of Ga@HAp; because of the material's absorption at 600 nm and its sedimentation during shaking and incubation the starting absorbances (optical densities, OD600) were subtracted and all the values are normalized to [0,1].

#### 1. Amino-acid-functionalized Au nanoparticles on a hydroxyapatite containing $Ga^{3+}$ ions (Au/amino acid@HAp(Ga))

The loading of hydroxyapatite with  $Ga^{3+}$  ions approaches saturation in about 24 hours and yields approximately 15 wt % of Ga(III) in hydroxyapatite, which is slowly released from the material during aging in PBS. We found that Au/amino acid@HAp(Ga) (Au/Arg@HAp(Ga), Au/Gly@HAp(Ga) and Au/His@HAp(Ga)) inhibit the growth of *Escherichia coli* MG1655.

#### 2. Ga nanoparticles on hydroxyapatite (Ga@HAp, Figure 3)

Gallium nanoparticles on hydroxyapatite are a new biomaterial with an antibacterial action. We found that it markedly inhibits the growth of *Pseudomonas aeruginosa* MW1 in PA01 (Figure 3). The diffusion antibiogram assay showed an inhibition zone around Ga@HAp, which contained no bacteria according to phase-contrast microscopy images (Figure 3, a and b). In a microdilution antibiogram of the suspension of the material we obtained minimal inhibition concentration (MIC) at 0.3 mg/mL, which in 24 h completely inhibited the growth of *P. aeruginosa* (Figure 3, d), while 0.4 mg/mL was the lowest concentration that effectively prevented the growth in 48 h. So far we have achieved such coverage of hydroxyapatite with Ga nanoparticles that approximately 15 wt % of Ga was in Ga@HAp. Although no major bactericidal effect was noticed, the live/dead fluorescence microscopy assay showed more agglomerates of dead bacteria for MIC of Ga@HAp than for the control (0 mg/mL or hydroxyapatite, Figure 3, c).

The application of vanadium pentoxide ( $V_2O_5$ ) as antibacterial material is limited by its reasonably high solubility in aqueous solutions. Because of that we developed a method to control the solubility of  $V_2O_5$  by the formation of 1D structures and their incorporation within a biocompatible polymeric matrix. Experimental results confirmed that by embedding vanadium pentoxide into the polymer matrix an efficient solubility control can be achieved. The elution of materials designed in such way provides vanadate within a concentration range known from the literature as bioactive. Moreover, test-

ing the interactions of the 1D nanostructured vanadium pentoxide with bacterial cells confirmed the inhibition of bacterial growth in a medium containing hydrogen peroxide. The main goal for future research in this field is to optimize the composite properties in order to combine both bioactive and antibacterial properties.

### Functionalized oxides for electronic applications

With a solid-state synthesis we prepared ceramic components based on nonstoichiometric sillenites, which contained  $M^{2+}$  ( $Co^{2+}$ ,  $Fe^{2+}$ ),  $M^{3+}$  ( $Ga^{3+}$ ,  $In^{3+}$ ) and  $M^{5+}$  ( $V^{5+}$ ) cations. We investigated their dielectric properties in the radio (<1 MHz) and microwave (4-6 GHz) frequency ranges. The results of the dielectric measurements in the radio-frequency range have shown that the dielectric constant decreases with the increasing valence of the  $M^{n+}$  cation in the sillenite ceramic, with values between 51 ( $Co^{2+}$ ) and 34 ( $V^{5+}$ ). The temperature coefficient of the dielectric constant changes from a pronounced negative -198 ppm/K ( $Co^{2+}$ ) to a highly positive 187 ppm/K ( $V^{5+}$ ). The microwave dielectric measurements also show a decrease in the dielectric constant from 57 ( $Co^{2+}$ ) to 35 ( $V^{5+}$ ) with an increase of the  $M^{n+}$  cation's valence, whereas the quality factor increases from 742 GHz ( $Co^{2+}$ ) to 1736 GHz ( $V^{5+}$ ). Suitable dielectric properties for further use in the electronics industry were obtained for a sillenite ceramic with  $Ga^{3+}$ , as its values are  $\epsilon \approx 40$ ,  $\tan\delta = 0.001$ ,  $\tau_k = 0$  ppm/K in the radio-frequency range (1MHz) and  $\epsilon \approx 47$ ,  $Q_{xf} = 1615$  GHz, and  $\tau_f = -11.65$  ppm/K in the microwave range (5 GHz).

In the scope of the MNT-ERA.NET project "Nanostructured ferroelectric films for biosensors" (Naferbio), which was coordinated by Prof. Spartak Gevorgian from Chalmers University of Technology, Sweden, we developed intrinsically tunable bulk acoustic wave resonators, based on sol-gel  $0.70Pb(Mg_{1/3}Nb_{2/3})O_3-0.30PbTiO_3$  (PMN-PT) thin films with a record high effective electromechanical coupling coefficient of 13% and a tunability of the series resonance frequency up to 4.0%. The enhanced electro-acoustic properties of the PMN-PT resonators were attributed to the mechanism of polarization rotation occurring in the region of the morphotropic phase boundary. In the study we analysed the electroacoustic performance of the PMN-PT resonators using the theory of dc field-induced piezoelectric effect in ferroelectrics, while the extrinsic acoustic losses in the PMN-PT resonators were analysed using a model of the wave scattering at reflections from rough interfaces. The mechanical  $Q$ -factor of the resonators totals up to 70 at 4.1 GHz and is limited mainly by losses in the PMN-PT film.

For the investigations of electroceramics with improved dielectric properties we focused on  $BaTiO_3$ . In order to prepare a densely sintered dielectric ceramic with submicron-sized grains, we investigated a sintering process for nanosized  $BaTiO_3$ . The research on  $BaTiO_3$  ferroelectric particles also included the (i) sintering of defined  $BaTiO_3$  particles and a determination of the dielectric properties of sintered ceramics and (ii) tailoring the shape, polarization and crystal orientation of plate-like ferroelectric particles. In the first part we studied the sintering of  $BaTiO_3$  particles, which according to a transmission electron microscope (TEM) examination, showed a square-like shape. The actual three-dimensional shape was neither an ideal cube nor an octahedron. The formed particles were not spherical and also not fully faceted. The development of the microstructure during sintering of these particles could be very interesting in terms of the mechanisms that control the grain growth. Depending on the driving force of the different mechanisms, the sintered ceramics consisted of normal growing grains, stagnant grains (growth rate is very low) or abnormal grains (liquid-phase sintering). Our investigations revealed that the relative contribution of a particular type of grains depended on the Ba:Ti ratio and sintering regime: two-step or isothermal sintering. The Ba:Ti ratio was controlled by the intensity of the acetic acid washing after the hydrothermal synthesis of the  $BaTiO_3$  powders. In the ceramics with Ba:Ti=1.01:1 and two-step sintering, stagnant grains prevailed, while normal grains in addition to stagnant and abnormal grains were present in the ceramics after the isothermal sintering. The former ceramics consisted of grains with an average grain size of 2  $\mu m$  and exhibited a higher dielectric constant ( $\epsilon$ ) and lower dielectric losses ( $\tan \delta$ ) at room temperature, compared to the isothermally sintered ceramics with an average grain size of 15  $\mu m$ . These ceramics exhibited a high dielectric constant of 11000 at the Curie temperature (121 °C). In the barium-deficient ceramics (Ba/Ti=0.98:1) a small amount of secondary  $Ba_6Ti_{17}O_{40}$  phase formed and the abnormal and stagnant grains dominated over the normal grains, which resulted in a low relative density (84-89 %) and a deterioration of the dielectric properties.

In the scope of the study of ferroelectric crystals with a defined shape, polarization and crystal orientation we dealt with the synthesis of  $Bi_{4-x}Nd_xTi_3O_{12}$  and  $BaTiO_3$  plates. The research was focused on the study of synthesis conditions, which enabled tailoring the size of the ferroelectric  $Bi_{4-x}Nd_xTi_3O_{12}$  ( $0 \leq x \leq 0.85$ ) plates and their topo-chemical transformation into  $BaTiO_3$  plates. Varying the synthesis conditions provides us with dimensional control of the  $Bi_{4-x}Nd_xTi_3O_{12}$  plates, from 100 nm to several microns in width, and from 20 nm to 100 nm in thickness. The influence of bismuth substitution with neodymium on the morphology of the  $Bi_{4-x}Nd_xTi_3O_{12}$  plates and their ferroelectric characteristics and domain structure was studied by means of electron microscopy, differential scanning calorimetry

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**The results of the study revealed, for the first time, an effective pathway for the preparation of a SrO-induced buffer layer on a silicon substrate using PLD, which can be subsequently utilized for the epitaxial growth of functional oxides.**

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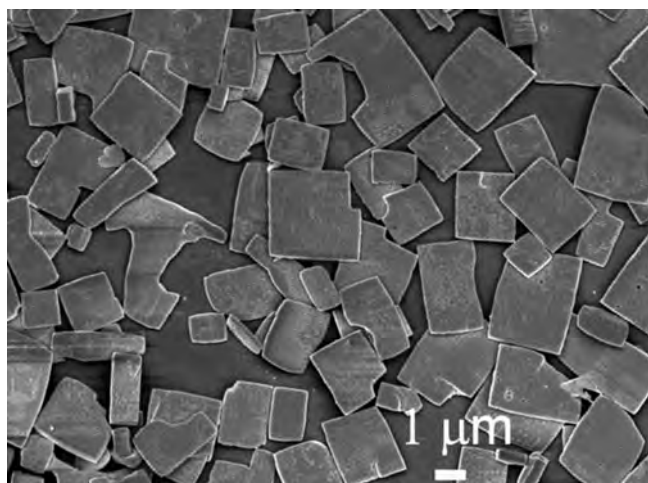


Figure 4: Ferroelectric tetragonal BaTiO<sub>3</sub> plates with a preferential (002) orientation.

**Funding was approved for the SCOPES project entitled "Intelligent Scaffolds as a Tool for Advanced Tissue Regeneration". The project is funded by the Swiss government, coordinated by a partner from ETH and includes two participants from Slovenia (IJS) and Serbia (TMF). For a period of three years we are going to investigate the formation of innovative bioactive and antibacterial nanomaterials, which will be incorporated within a porous polymeric matrix to form stable scaffolds and will be later on tested for interactions with human stem cells.**

(DSC) and piezo-force microscopy (PFM). DSC analyses revealed the decrease of the Curie temperature by 40°C when  $x$  changed from  $x=0$  to  $x=0.2$ . The PFM investigations showed the presence of irregularly shaped ferroelectric domains and polarization in the plane of the Bi<sub>3.8</sub>Nd<sub>0.2</sub>Ti<sub>3</sub>O<sub>12</sub> plate.

The dimensions, crystal structure and orientation of the single-crystalline BaTiO<sub>3</sub> plates, which were topo-chemically converted from the Bi<sub>4-x</sub>Nd<sub>x</sub>Ti<sub>3</sub>O<sub>12</sub> plates, were controlled by the template size, the composition and by the conversion conditions. Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub>-based plates mainly led to (002)-oriented tetragonal BaTiO<sub>3</sub> plates (Figure 4), whereas Bi<sub>4-x</sub>Nd<sub>x</sub>Ti<sub>3</sub>O<sub>12</sub> ( $0.2 \leq x < 0.85$ ) favoured (200)-oriented cubic BaTiO<sub>3</sub> plates. In this study we faced the challenge of preparing highly tetragonal (002)-oriented BaTiO<sub>3</sub> plates that are considerably less than 1 μm in width and less than 100 nm in thickness. The development of such ferroelectric plates is of great interest in the study of ferroelectric behaviour on the nanoscale and for the realization of miniaturized ferroelectric devices by assembling their plates.

The investigations of the ferroelectric particles with a defined shape were performed in the scope of INNOINKS (MATERA-ERA-NET) project in cooperation with the Microelectronics and Materials Physics Laboratories (University of Oulu, Finland), the Institute of Electronic Materials Technology (Poland), Sachtleben Pigments Oy, Pulse Finland Oy and the NOF Corporation (Japan). The continuation of the research, which is focused on the tailoring of the polarization and crystal orientation of ferroelectric plates, is now going on in the framework of the ARRS projekt: Engineering of structural and microstructural characteristics in contemporary dielectrics and ferroelectrics with perovskite and perovskite-like crystal structures.

The perovskite structure of piezoelectrics has been extensively studied due to the intrinsic (structural) contribution to enhanced piezoelectric effects. For defined compositions of the piezoelectric solid solutions the morphotropic phase boundaries (MPBs) form, where the electromechanical properties reach the highest values. Our research was based on determining the crystal structure at the MPB in the (Na<sub>1-x</sub>K<sub>x</sub>)<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> solid solution system (at  $x = 0.2$ ). From a detailed structural analyses of the MPB material by XRD and *in-situ* TEM it was concluded that the crystal structure in its virgin state is pseudocubic, with no preferential lattice orientations. It actually becomes morphotropic (i.e., with two or more structures coexisting) after the material is subjected to external forces (e.g., grinding, polishing, poling, etc.). Depending on the type of sample treatment the structure of the crystal lattice evolves with a tetragonal symmetry, with a rhombohedral one, or with the

coexistence of both symmetries. A large benefit of such behaviour is that the lattice of the as-prepared material has almost no restrictions with respect to the direction of the lattice deformation upon the application of external fields. Thus, large piezoelectric effects are observed at MPBs.

The work was also directed to the synthesis of cobalt ferrite nanoparticles (CFO). We investigated the effect of oleic acid concentration on the physicochemical properties of solvothermally derived cobalt ferrite nanoparticles (CFO). Without the oleic acid, agglomerated nanoplatelets with a crystallite size of about 19 nm were obtained, according to the X-ray diffraction and transmission electron microscopy. However, the addition of oleic acid decreases the size of the CFO nanoparticles and at critical concentration, which was determined to be 0.25 M, well-dispersed, non-agglomerated spherical particles of about 6 nm were obtained. A further increase in the oleic acid concentration affected the particle size only slightly, with a relatively constant surface coverage of the oleic acid ligand.

The results of our study indicate that particle-size control was achieved by bridging bidentate interactions between the oleic acid molecules and the metal atoms on the surface of the nanoparticles, as determined by Fourier transform infrared spectra. These interactions affected the surface strain of the nanoparticles considerably, but kept the initial cation redistribution according to the Raman spectra. The room-temperature magnetic measurements revealed that oleic acid enables us to effectively control the magnetic behaviour of the CFO, which changes from ferrimagnetic to superparamagnetic at a critical concentration. Interparticle interactions are further

interpreted using low-temperature magnetic measurements, which also showed a decreased surface anisotropy for the samples prepared with an oleic acid concentration above the critical value. An investigation of the treatment

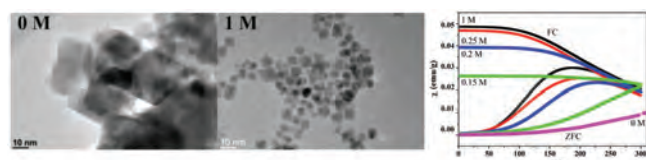


Figure 5: TEM images of CFO nanoparticles synthesized with 0- and 1-M oleic acid concentration. Low-temperature measurements of the particles' susceptibility versus the oleic acid concentration.



time showed that the capping with oleic acid is already achieved after 1 h of synthesis, but in order to improve the crystallization and consequently achieve the desired magnetic response a synthesis time of at least 4 h is required.

With our research on thin-film synthesis using pulsed-laser deposition (PLD) we focused on the epitaxial integration of strontium titanate ( $\text{SrTiO}_3$ ) with silicon (Si). Epitaxial  $\text{SrTiO}_3$  (STO) on Si serves as an excellent template layer and thus enables various functional oxide thin films to be integrated in the epitaxial form with silicon substrates. We started with an investigation of both thermal and strontium-induced deoxidation processes for the elimination of the native  $\text{SiO}_2$  from the Si surface. The aim was to prepare a surface, appropriate for the further deposition of the strontium (Sr) buffer layer, which is based on  $\frac{1}{2}$  ML of Sr coverage. High-temperature annealing ( $T > 1100^\circ\text{C}$ ) proved to be the most efficient deoxidation process, since the  $\beta$ -SiC islands that form on the Si surface either during thermal or Sr-assisted deoxidation, can easily be dissociated at such a high temperature. Additionally, we showed the ability to prepare highly-ordered sub-monolayer structures of Sr on a Si surface with the PLD method. Using the reflection high-energy electron diffraction (RHEED) technique we observed characteristic two-domain  $(2 \times 3) + (3 \times 2)$  pattern at  $\frac{1}{6}$  ML Sr coverage and  $(1 \times 2) + (2 \times 1)$  pattern at  $\frac{1}{2}$  ML Sr coverage. The  $\frac{1}{2}$  ML of Sr on Si acts as an effective passivation layer, which is a prerequisite for the successful epitaxial growth of the STO layer. By means of X-ray photoelectron spectroscopy (XPS) and X-ray reflectivity (XRR) we determined very critical initial parameters for the STO deposition by the method of kinetically controlled sequential deposition (KCS). Based on the RHEED and X-ray diffraction results (XRD), it is concluded that STO is epitaxially grown on Si with an out-of plane relationship of  $\text{STO}(001) \parallel \text{Si}(001)$  and an in-plane relationship of  $\text{STO}[110] \parallel \text{Si}[100]$ . Because of the recent commercialization of large-area PLD systems we believe the results of our work are very relevant for implementation of oxide electronics integrated with Si platform and bring in an alternative manufacturing route.

The epitaxial growth of functional oxides on silicon substrates requires atomically defined surfaces, which are most effectively prepared using Sr-induced deoxidation. The manipulation of metallic Sr is nevertheless very delicate and requires alternative buffer materials. In our study the applicability of the chemically much more stable SrO in the process of native-oxide removal and silicon-surface stabilization was investigated using the PLD technique, while the as-derived surfaces were analysed in-situ using RHEED and ex-situ using XPS, XRR and atomic force microscopy. After the deposition of the SrO over  $\text{Si}/\text{SiO}_2$ , in a vacuum, different annealing conditions, with the temperature ranging up to  $850^\circ\text{C}$ , were applied. Due to the deposition taking place in a vacuum a multilayer composed of SrO,  $\text{SrSiO}_3$ , modified Si, and Si as a substrate was initially formed. During the subsequent annealing the topmost layer epitaxially orders in the form of islands, while a further increase in the annealing temperature induced rapid desorption and surface deoxidation, leading to a  $2 \times 1$  Sr-reconstructed silicon surface. The results of the study revealed, for the first time, an effective pathway for the preparation of a SrO-induced buffer layer on a silicon substrate using PLD, which can be subsequently utilized for the epitaxial growth of functional oxides.

The project "Thin-Film-Energy-Storage Devices on the basis of PLZT and Cu-electrodes" with industrial partner EPCOS OHG, Deutschlandsberg, Austria, focuses on the solid-state chemistry of zirconium-rich  $\text{Pb}_{(1-x)}\text{La}_x(\text{Zr}_y\text{Ti}_{(1-y)})\text{O}_3$  (PLZT), as well as the growth of PLZT thin films using pulsed-laser deposition. The purpose of the project is to develop new materials and technologies for advanced energy-storage applications. With the cooperation of the industrial partner Knauf Insulation d.o.o, the research work on the joint project was focused on mineral fibres and their composites. We have worked on research subjects such as the composition and melting behaviour of raw materials, the influence of the aging process on the morphology and composition of mineral fibres, the specific heat and enthalpy change determination of glass melts, the thermal stability of mineral wools, binders and gypsum boards and the synthesis of new composites materials based on mineral fibres with improved insulation properties.

## Some outstanding publications in the past year

1. Vukomanović, M., Logar, M., Škapin, S. D., Suvorov, D.: Hydroxyapatite/gold/arginine : designing the structure to create antibacterial activity. *Journal of materials chemistry. B, Materials for biology and medicine*, 2014, vol. 2014, issue 11, 1557-1564, doi: 10.1039/C3TB21612H
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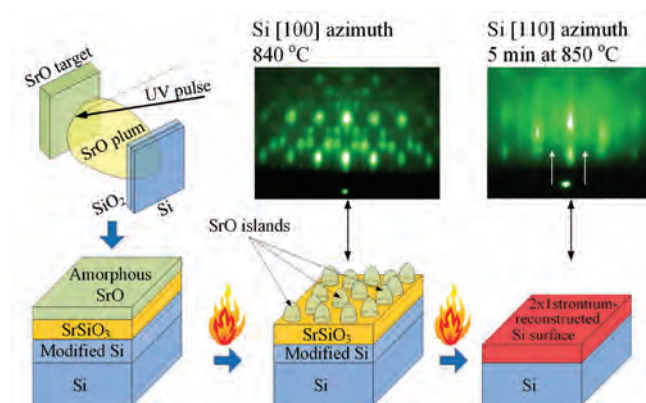


Figure 6: Schematics of SrO-induced surface deoxidation and reconstruction of Si surface using a PLD technique.



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- Li, L., Spreitzer, M., Suvorov, D.: Unique dielectric tunability of  $\text{Ag}(\text{Nb}_{(1-x)}\text{Ta}_x)\text{O}_3$  ( $x=0-0.5$ ) ceramics with ferroelectric polar order. *Applied physics letters*, ISSN 0003-6951. [Print ed.], 2014, vol. 104, no. 18, str. 182902-1-182902-5, doi: 10.1063/1.4875581.
- Jovanović, S., Spreitzer, M., Tramšek, M., Trontelj, Z., Suvorov, D.: Effect of oleic acid concentration on the physicochemical properties of cobalt ferrite nanoparticles. *The journal of physical chemistry: C, Nanomaterials and interfaces*, ISSN 1932-7447, 2014, vol. 118, issue 25, str. 13844-13856, doi: 10.1021/jp500578f.

## INTERNATIONAL PROJECTS

- Thin-Film-Energy-Storage Device on the basis of PLZT and Cu-Electrodes  
Prof. Danilo Suvorov  
EPCOS OHG
- Technological Characterisation Test of OGC-5 (RGRES) Ashes for Verification of Usability in the Process of Rock Wool Production  
Prof. Danilo Suvorov  
Enel Ingegneria e Ricerca S.p.A
- Microwave Tunable Materials, Composites and Devices  
Asst. Prof. Boštjan Jančar  
NATO - North Atlantic Treaty Organisation
- Multifunctional Ferroelectric Materials based on  $\text{Ag}(\text{Nb,Ta})\text{O}_3$   
Prof. Danilo Suvorov  
Slovenian Research Agency
- Biomaterialization at the Nanoscale: From the Natural Systems to the Laboratory  
Asst. Prof. Srečo Davor Škapin  
Slovenian Research Agency
- 3D Composite Plasmonic Metal/Semiconductor Photo-catalyst for Efficient Solar to Fuel Energy Conversion  
Dr. Manca Logar  
Slovenian Research Agency

## R & D GRANTS AND CONTRACTS

- Nanoengineering of Self-assembled Materials  
Prof. Danilo Suvorov
- Engineering of Structural and Microstructural Characteristics in Contemporary Dielectrics and Ferroelectrics with Perovskite and Perovskite-like Crystal Structures  
Prof. Danilo Suvorov
- Growth of High Quality Piezoelectric Thin Films on Silicon using Pulsed Laser Deposition  
Dr. Matjaž Spreitzer
- New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics  
Prof. Danilo Suvorov
- INNOINKS: Novel Inorganic Inks for Hybrid Printed Electronic Demonstrators  
Prof. Danilo Suvorov
- NAFERBIO: Nanostructured Ferroelectric Films for Biosensor  
Prof. Danilo Suvorov
- Enabling Technology for High-quality piezoMEMS  
Dr. Matjaž Spreitzer
- SCOPE5: Intelligent Scaffolds as a Tool for Advanced Tissue Regeneration  
Dr. Marija Vukomanović

## RESEARCH PROGRAM

- Contemporary Inorganic Materials and Nanotechnologies  
Prof. Danilo Suvorov

## NEW CONTRACT

- Development and Characterisation of Mineral Wool Fibres  
Prof. Danilo Suvorov

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29. Marija Vukomanović, Manca Logar, Srečo D. Škapin, Danilo Suvorov, "Hydroxyapatite/gold/arginine: designing the structure to create antibacterial activity", *J. mater. chem. B*, vol. 2014, issue 11, pp. 1557-1564, 2014.
30. Vojka Žunič, Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, Janez Kovač, "Photocatalytic properties of TiO<sub>2</sub> and TiO<sub>2</sub>/Pt: a sol-precipitation, sonochemical and hydrothermal approach", *Ultrason. sonochem.*, vol. 21, issue 1, pp. 367-375, 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. A. Suslov, Dmitrii Durilin, Oleg V. Ovchar, Anatolii Belous, Viktor Bovtun, Martin Kempa, Boštjan Jančar, Matjaž Spreitzer, "Synthesis and dielectric properties of BaTi<sub>1-x</sub>ZrxO<sub>3</sub> -based ceramic and film materials", In: *ELNANO 2014*, 34th International Conference on Electronics and Nanotechnology, 15 April - 18 April 2014, Kyiv, Ukraine, Kyiv, National Technical University of Ukraine Kyiv Polytechnic Institute Polytekhchna, 2014, pp. 66-69.

## PATENT APPLICATION

1. Boštjan Jančar, Damjan Vengust, Danilo Suvorov, *Thermoelectric ceramic materials and generators made thereof*, EP14177502.3, European Patent Attorneys, 2014.
2. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, *A method to produce foam glasses*, 53861DK01, Danish Patent and Trademark Office, 7.7.2014.

## MENTORING

1. Sonja Jovanović, *Synthesis of cobalt ferrite nanoparticles and their embedding into magnetoelectric composite film via block co-polymer self-assembly*: doctoral dissertation, Ljubljana, 2014 (mentor Danilo Suvorov; co-mentor Matjaž Spreitzer).
2. Mojca Otoničar, *Intragranular nanostructure of the (Na<sub>1-x</sub>K<sub>x</sub>)<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> perovskite solid solutions*: doctoral dissertation, Ljubljana, 2014 (mentor Srečo D. Škapin; co-mentor Boštjan Jančar).
3. Vojka Žunič, *Synthesis and characterization of TiO<sub>2</sub> nano-powders and TiO<sub>2</sub>/Pt nano-composites for photocatalytic applications*: doctoral dissertation, Ljubljana, 2014 (mentor Danilo Suvorov; co-mentor Srečo D. Škapin).
4. Vladimira Petrovič, *High temperature application of nano TiO<sub>2</sub> on the ceramic substrate and determination of the photocatalytic efficiency*: master's thesis, Ljubljana, 2014 (mentor Srečo D. Škapin; co-mentor Vilma Ducman).



# 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. Part of the activities is devoted to the development of tools that allow us to understand the properties of proteases and other enzymes, as well as to enable their monitoring and manipulation in *in vivo* conditions.**

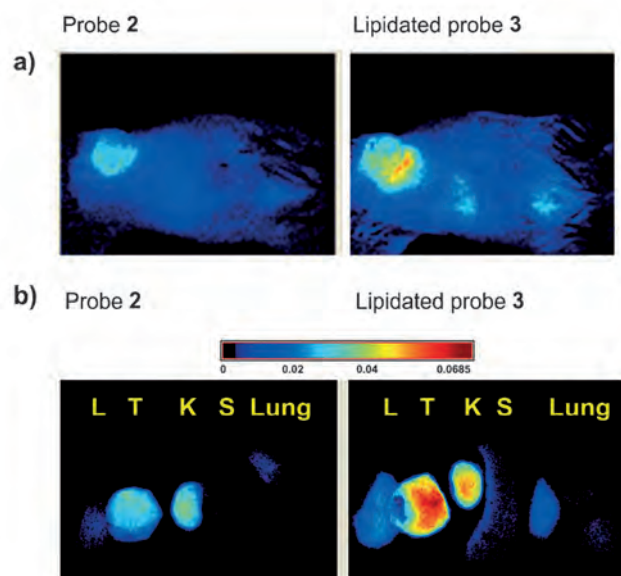
Protease research has undergone a major expansion in the past decade, largely due to the extremely rapid development of new technologies, such as quantitative proteomics and *in vivo* imaging, as well as an extensive use of *in vivo* models. These have led to the identification of physiological substrates and resulted in a paradigm shift from the concept of proteases as protein-degrading enzymes to proteases as key signalling molecules. Their catalytic activities are precisely regulated, the most important ways being zymogen activation and inhibition by their endogenous protein inhibitors. Any imbalance of this regulation can lead to pathologies such as autoimmune, neurological and cardiovascular disorders, cancer and osteoporosis. However, protease signalling pathways are only partially understood. Currently, only a minor subset of physiological substrates for a limited number of proteases has been identified, and their physiological regulation is still not well understood.

A significant amount of work has been done on understanding protease function in health and disease with a major focus on cancer. It has been known for a long time that cysteine cathepsins, in particular cathepsins B, L and S, play a major role in cancer progression. One way how to address their function is through the development of imaging tools that allow for whole-body imaging and the precise detection of tumors *in vivo*, and represents an important part of chemical biology nowadays. There are two major principles, i.e., covalent activity-based probes and substrate-like FRET probes. The latter can largely amplify the signal, but suffer from the rapid clearance from the site of action. Using the concept of reverse design and optimized nonpeptidic inhibitor as the scaffold, we introduced a lipidated, non-peptidic FRET probe for cathepsin S, a protease secreted by macrophages in the tumor environment. We have shown that in cultured cells, as well as in a grafted tumor mouse model, the probe was successfully cleaved and in the mouse was accumulated in the tumor tissue with little signal in organs such as liver and lung (Figure 1). The probe is therefore a highly promising prototype tool for detecting tumors in humans in the future and can also serve as a very valuable tool in validating cathepsin S targeting compounds *in vivo*. In addition, we focused on cathepsin B, a lysosomal cysteine proteinase that is specifically translocated to the extracellular milieu during cancer progression. We therefore developed a lipidated cathepsin B inhibitor and incorporated it into the envelope of a liposomal nanocarrier (LNC-NS-629). *Ex vivo* and *in vivo* studies confirmed the selective targeting and internalization of LNC-NS-629 by tumor and stromal cells. Moreover, when incorporated in this liposomal nanocarrier, the anticancer drug doxorubicine was found to be much more potent in killing primary cancer cells than the non-targeted doxorubicine encapsulated in liposomes, thus validating cathepsin B targeting as a highly promising approach to cancer diagnosis and treatment. Furthermore, this novel concept represents a paradigm shift in protease research, as targeting a protease was for the first time used for targeted drug delivery and not for therapeutic inhibition of the protease activity (Figure 2, 3).

Another protease that we focused on was cathepsin K, which is a major target in osteoporosis treatment. In collaboration with colleagues from the Faculty of Chemistry and Chemical Technology and Switzerland (A. Baici) we developed a procedure for allosteric site prediction in papain-like cysteine peptidases using computational methods, using cathepsin K as the model enzyme. Compound libraries were screened *in silico* to identify the compound NSC13345 as the first low-molecular-weight allosteric inhibitor of cathepsin K. The compound was thoroughly characterized from the functional and structural perspectives. The crystal structure of the cathepsin K/NSC13345



Head:  
**Prof. Boris Turk**



**Figure 1: Whole body imaging of cathepsin S in a mouse tumour model. (a) Whole-mouse optical images of 4T1 tumour-bearing mice at 24 hours post *i.v.* injection of non-lipidated (2, left) and lipidated (3, right) probes, respectively ( $n = 5$ ). (b) Distribution of probes 2 and 3 in key organs at 5 days post injection.**



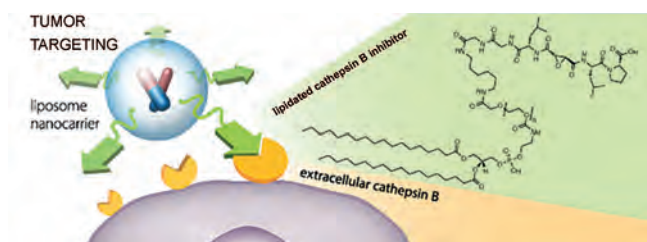


Figure 2: A lipitated cathepsin B (CtsB) inhibitor was incorporated into the envelope of a liposomal nanocarrier. The resulting CtsB-targeted drug delivery system, which can be loaded with diagnostic or therapeutic agents, was selectively internalized by tumour and stromal cells, thus validating CtsB targeting as a promising approach to cancer diagnosis and treatment.

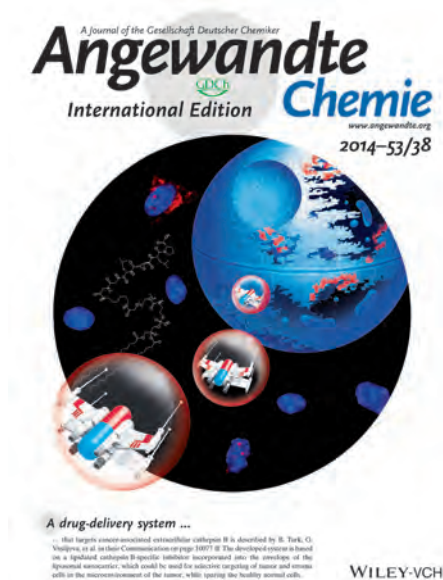


Figure 3: Inside back cover image of *Angewandte Chemie International Edition*.

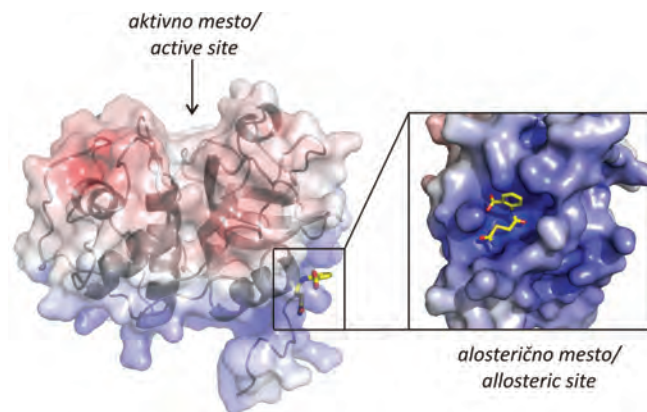


Figure 4: Crystal structure of cathepsin K with the compound NSC13345 (shown as sticks) bound to an allosteric site. This is the first example of a low-molecular-weight allosteric effector of cysteine cathepsins.

complex showed that the compound indeed binds at the computationally anticipated site, which was thereby identified as a novel allosteric site in cathepsin K. The compound was characterized as a partial inhibitor of the hydrolysis of synthetic substrates and azocasein and a full inhibitor of type-I collagen hydrolysis. These results qualify compound NSC1334 as an excellent candidate for the design of drugs for the treatment of osteoporosis (Figure 4).

We also worked on the identification of protease substrate specificities and on the development of proteomic methods for their identification. With K. Gevaert (University of Ghent) we successfully developed one such new method termed Fast Profiling of Protease Specificity (FPPS) that was successfully applied to cathepsins K, L and S, and was found to give similar results as COFRADIC, one of the major approaches used in determining the substrate specificities of proteases. FPPS could thus serve as a complementary

strategy to other well-established proteomic methods. Another important achievement was the determination of the crystal structure of the epithelial cell adhesion molecule (EpcAM), a cell surface protein and a stem and carcinoma cell marker involved in homotypic cell-cell adhesion via intercellular oligomerization and proliferative signalling via proteolytic cleavage and further characterization of the proteolytic processing. Since EpcAM is closely related to other CAM molecules, which we identified to be shed by cysteine cathepsins L and S, this finding may have further implications in our understanding of cancerous processes. The work was performed in collaboration with the Faculty of Chemistry and Chemical Technology and the University of Vienna (K. Djinovic Carugo). Another important achievement in the area of structural biology was the determination of the partial rotational lattice order-disorder in crystals of stefin B, a major intracellular inhibitor of cathepsins. At present, the determination of crystal structures from data that have been acquired from twinned crystals is routine; however, with the increase of crystal structures, additional crystal-lattice disorders are discovered. We identified a previously undescribed, partial rotational order-disorder that has been observed in the crystals of stefin B. The diffraction images reveal normal diffraction patterns that result from a regular crystal lattice; however, one crystal exhibited a notable rejection rate in the higher symmetry space group. In this work we further showed how it is possible to identify and successfully deal with such crystal-lattice disorders.

In addition, we have continued to develop computational approaches for crystallography. One such approach is the refinement of a molecular model, a computational procedure by which the atomic model is fitted to the diffraction data. The commonly used target in the refinement of macromolecular structures is the maximum-likelihood (ML) function, which relies on the assessment of model errors. The current ML functions rely on cross-validation. They utilize phase-error estimates that are calculated from a small fraction of the diffraction data, called the test set, that are not used to fit the model. An approach has been developed that uses the work set to calculate the phase-error estimates in the ML refinement from simulating the model errors via the random displacement of atomic coordinates. It is called ML free-kick refinement as it uses the ML formulation of the target function and is based on the idea of freeing the model from the model bias imposed by the chemical energy restraints used in the refinement. This approach for the calculation of error estimates is superior to the cross-validation approach: it reduces the phase error and increases the accuracy of molecular models, is more robust, provides clearer maps and may use a smaller portion of the data of the test set for the calculation of R<sub>free</sub> or may leave it out completely, which has been designed to interactively perform the complex tasks of macromolecular crystal structure determination and validation.

Our department has, partially through the help of the Center of Excellence for Integrative approaches for Chemistry and Biology of Proteins (CIPKEBIP), established several technological platforms that are all unique in Slovenia and include a structural biology platform, proteomics platform and a whole-body imaging platform, based on the IVIS Spectrum imaging system. All three platforms are open for external collaborations and several works resulting from these collaborations have already been published.

We participated in the FP7 project Alexander and were also involved in the Slovenian Center of Excellence CIPKEBIP, which we also coordinate. We were partners in the competence center BRIN, which, similar to the Centers of Excellence, brings together researchers from both industry and academia.

In addition, there are numerous other international collaborations with excellent research teams from different countries, including Belgium (a joint project through FWO), France, Germany, Sweden, Switzerland, UK, USA, Australia and Japan, which resulted in joint publications.

In addition, prof. dr. Boris Turk received the Lapanje Award for outstanding scientific achievements in the field of proteolysis, which is given by Slovene Biochemical Society. Several members of the department were invited to give lectures at international symposia and foreign universities.

### Some outstanding publications in the past year

1. Mikhaylov, G., Klimpel, D., Schaschke, N., Mikac, U., Vizovišek, M., Fonovič, M., Turk, V., Turk, B. \*, Vasiljeva, O. \* (2014): Selective targeting of tumor and stromal cells by a nanocarrier system displaying lipidated cathepsin B inhibitor. *Angew Chem Int Ed Engl.*, 53 (38), 10077–10081 (shared last\* authors)
2. Hu, Hy\*, Vats, D. \*, Vizovišek, M. \*, Kramer, L., Germanier, C., Wendt, K., Rudin, M., Turk, B. \*\*, Plettenburg, O. \*\*, Schultz, C. \*\* (2014): *In vivo* imaging of mouse tumors by a lipidated cathepsin S substrate. *Angew Chem Int Ed Engl.*, 53 (29), 7669–7673 (shared first\* and last\*\* authors)
3. Novinec, M., Korenč, M., Caflisch, A., Ranganathan, R., Lenarčič, B., Baici, A. (2014): A novel allosteric mechanism in the cysteine peptidase cathepsin K discovered by computational methods. *Nat Commun*; 5:3287, doi: 10.1038/ncomms4287
4. Pavšič, M., Gunčar, G., Djinović-Carugo, K., Lenarčič, B. (2014): Crystal structure and its bearing towards an understanding of key biological functions of EpCAM. *Nat Commun.*; 5:4764, doi: 10.1038/ncomms5764
5. Pražnikar, J., Turk, D. (2014): Free kick instead of cross-validation in maximum-likelihood refinement of macromolecular crystal structures. *Acta Crystallogr D Biol Crystallogr.*; 70 (Pt 12), 3124–3134
6. Renko, M., Taler-Verčič, A., Mihelič, M., Žerovnik, E., Turk, D. (2014): Partial rotational lattice order-disorder in stefin B crystals. *Acta Crystallogr D Biol Crystallogr.*, 70 (Pt 4), 1015–1025

### Awards and appointments

1. Boris Turk: Lapajne award for outstanding scientific achievements in the field of proteolysis, Slovenian Biochemical Society, Ljubljana, Slovenia
2. Vito Turk: appointment to the Russian Engineering Academy, Wien, Austria
3. Vito Turk: Zois award for life work, Ministry of Education, Science and Sport, Ljubljana, Slovenia

### Organisation of conferences, congresses and meetings

1. 31<sup>st</sup> Winter School on Proteases and their Inhibitors, Tiers, Italy, 26 February–2 March 2014 (co-organisers)
2. XIV<sup>th</sup> International Symposium on Proteinases, Inhibitors and Biological Control, Portorož, Slovenia, 6–10 September 2014 (organisers)

### Patent

1. Marko Šnajder, Nataša Poklar Ulrih, Marko Mihelič, Dušan Turk, Overproducing recombinant form of pennisine in heterologous expression system, SI24364 (A), Urad RS za intelektualno lastnino, 28.11.2014.

## INTERNATIONAL PROJECTS

1. Supply of DPPI Enzyme and the Non-exclusive License Rights  
Prof. Dušan Turk  
Prozymex A/s
2. 7FP - ALEXANDER; Mucus Permeating Nanoparticulate Drug Delivery Systems  
Asst. Prof. Olga Vasiljeva  
European Commission
3. COST BM1307; European Network to Integrate Research on Intracellular Proteolysis Pathways in Health and Disease (PROTEOSTASIS)  
Prof. Boris Turk  
COST Office
4. The Association Between Breast Cancer and Cathepsins and its Related Gene Expression  
Prof. Vito Turk  
Slovenian Research Agency
5. Protective Role of Cystatins in LPS Induced Oxidative Stress and Sepsis  
Asst. Prof. Nataša Kopitar – Jerala  
Slovenian Research Agency

## RESEARCH PROGRAMS

1. Structural Biology  
Prof. Dušan Turk
2. Proteolysis and its Regulation  
Prof. Boris Turk

## R & D GRANTS AND CONTRACTS

1. The Role of Cysteine Cathepsins in Cellular Signalling  
Prof. Boris Turk
2. Cell Signalling of Toll-like Receptors  
Asst. Prof. Nataša Kopitar – Jerala
3. Role and Relevance of Empirical Geometric Parameters in Crystal Structure Determination of Macromolecules for Prediction of Ligand Binding  
Prof. Dušan Turk
4. Role of Cysteine Proteases in the Process of Cancerogenesis  
Asst. Prof. Marko Fonovič

5. Integrative Research of Sexual Dimorphism Evolution  
Prof. Boris Turk
6. The Role of Small GTPases in the Regulation of Endosomal/Lysosomal Transport in Astrocytes  
Prof. Veronika Stoka
7. Secretory Vesicle Mobility and Calcium Homeostasis in Astrocytes  
Prof. Veronika Stoka
8. Involvement of the Lysosomal Cysteine Peptidase Inhibitors in Progression and Metastasis of Mammary Cancer  
Asst. Prof. Olga Vasiljeva
9. Inhibitors of Cysteine Carboxypeptidases as Regulators of Autoimmune and Neurodegenerative Processes  
Asst. Prof. Olga Vasiljeva
10. Study of Hom(e)ologous Recombination in the Evolution of Polyketide Synthases  
Prof. Boris Turk
11. Nitroxoline and its Derivatives as New Antitumour Drugs  
Asst. Prof. Olga Vasiljeva
12. Oligomers of Amyloidogenic Proteins from A to Z: Biophysical Properties, Structure, Function and Mutual Interactions  
Prof. Eva Žerovnik
13. Research on New Technologies for Conservation – Restoration of Baroque Easel Paintings  
Asst. Prof. Marko Fonovič
14. XIVth International Symposium on Proteinases, Inhibitors and Biological Control, Portorož, Slovenia, 6-10 September 2014  
Prof. Boris Turk
15. Cellular Evaluation of Nanofibres  
Prof. Boris Turk
16. Competency Centre for Biotechnological Development and Innovation: CC BDI  
Prof. Boris Turk
17. Lysosomotropic Agents and Polyketide Compounds as Potential Therapeutics for Cancer Treatment  
Dr. Maruša Hafner Česen

## NEW CONTRACT

1. Mass spectrometry analysis  
Prof. Boris Turk  
Krka, Tovarna zdravil, d. d.

## VISITORS FROM ABROAD

1. Georgy Mikhaylov, Siberian State Medical University, Tomsk, Siberia, Russia, 1 January–31 September 2014 (IJS fellowship holder)
2. Andrey Kadin, Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Science, Moscow, Russia, 1 January–31 December 2014 (IJS fellowship holder)
3. Emilio Parisini, PhD, Center for Nano Science and Technology (CNST), Italian Institute of Technology (IIT), Milan, Italy, 6 February 2014
4. Prof. Guido Kroemer, INSERM U848, Institut Gustave Roussy, Villejuif, France, 23–24 March 2014
5. Dr. Maria Leptin and Dr. Gerlind Wallon, EMBO, Heidelberg, Germany, 15–16 April 2014
6. Prof. Kazuo Umezawa, Department of Molecular Target Medical Screening, School of Medicine, Aichi Medical University, Nagakute, Japan, 6–9 October 2014

## STAFF

### Researchers

1. Dr. Iztok Dolenc
2. Asst. Prof. Marko Fonovič
3. Asst. Prof. Nataša Kopitar - Jerala
4. Prof. Brigita Lenarčič\*
5. Asst. Prof. Urška Repnik
6. *Abelardo Manuel Silva, B. Sc., left 01. 07. 14*
7. Prof. Veronika Stoka
8. Andrej Šali, B. Sc.
9. **Prof. Boris Turk, Head**
10. Prof. Dušan Turk
11. Prof. Vito Turk
12. Dr. Livija Tušar
13. Asst. Prof. Olga Vasiljeva
14. Asst. Prof. Tina Zavašnik Bergant
15. Prof. Eva Žerovnik

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16. Dr. Miha Butinar
17. Dr. Mirjam Fröhlich
18. Dr. Maruša Hafner Česen
19. Dr. Georgy Mikhaylov
20. *Dr. Petra Nikolič, left 01. 07. 14*
21. Dr. Katarina Pegan
22. *Dr. Cristina Gabriela Pinto Droga Mazovec, left 01. 07. 14*
23. Dr. Jure Pražnikar\*
24. *Dr. Miha Renko, left 01. 07. 14*
25. Dr. Ajda Taler-Verčič
26. Dr. Aleksandra Usenik
27. Dr. Matej Vizovišek

### Postgraduates

28. Teja Bajt, B. Sc.
29. Katja Bidovec, B. Sc.
30. Janja Božič, B. Sc.
31. Katarina Hočevar, B. Sc.
32. Barbara Jerič Kokelj, B. Sc.
33. Aleksander Krajnc, B. Sc.
34. Lovro Kramer, B. Sc.
35. Sabina Ott, B. Sc.
36. Sara Pintar, B. Sc.
37. Jelena Rajković, B. Sc.
38. Mojca Trstenjak Prebanda, B. Sc.
39. Robert Vidmar, B. Sc.
40. Janja Završnik, B. Sc.

### Technical officers

41. *Andrejka Doberšek, B. Sc., died 18. 11. 14*
42. Dr. Vida Puizdar
43. Andreja Sekirnik, B. Sc.
44. Barbara Sobotič, B. Sc.
45. Ivica Štefe, B. Sc.

### Technical and administrative staff

46. *Louisa Johanna Kroon Žitko, B. Sc., retired 01. 09. 14*
47. Maja Orehek, B. Sc.
48. Dejan Pelko
49. Polonca Pirš Kovačič
50. Barbara Vrtačnik

Note:

\* part-time JSI member



# BIBLIOGRAPHY

## ORIGINAL ARTICLE

- Petra Avanzo Caglič, Miha Renko, Dušan Turk, Janko Kos, Jerica Sabotič, "Fungal  $\beta$ -trefoil trypsin inhibitors cnispin and cospin demonstrate the plasticity of the  $\beta$ -trefoil fold", *Biochimica et biophysica acta, Proteins and proteomics*, vol. 1844, issue 10, pp. 1749-1756, 2014.
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- Katarina Maher, Barbara Jerič, Miha Butinar, Georgy Mikhaylov, Mateja Manček Keber, Veronika Stoka, Olga Vasiljeva, Boris Turk, Sergei A. Grigoryev, Nataša Kopitar-Jerala, "A role for stefin B (cystatin B) in inflammation and endotoxemia", *J Biol Chem*, vol. 289, no. 46, pp. 31736-31750, 2014.
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- Marko Novinec, Brigita Lenarčič, Antonio Baici, "Probing the activity modification space of the cysteine peptidase cathepsin K with novel allosteric modifiers", *PLoS one*, vol. 9, no. 9, art. no. e106642 (str. 1-11), 2014.
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## SHORT ARTICLE

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1. Marjana Novič, Livija Tušar, Marjan Tušar, Jure Zupan, "Structural elucidation", In: *Reference module in chemistry, molecular sciences and chemical engineering*, Jan Reedijk, ed., Oxford, Elsevier, 2014, 11 pp.
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3. Eva Žerovnik, "On possible function and toxicity of multiple oligomeric/conformational states of a globular protein human stefin B", In: *Bio-nanoimaging: protein misfolding & aggregation*, Vladimir N. Uversky, ed., Yury Lyubchenko, ed., Amsterdam [et al.], Elsevier, 2014, pp. 263-270.

## PATENT

1. Marko Šnajder, Nataša Poklar Ulrih, Marko Mihelič, Dušan Turk, *Overproducing recombinant form of pernissine in heterologous expression system*, SI24364 (A), Urad RS za intelektualno lastnino, 28.11.2014.

## MENTORING

1. Miha Butinar, *The role of stefin B and cystatin C in tumorigenesis in transgenic mouse mammary cancer model*: doctoral dissertation, Ljubljana, 2014 (mentor Boris Turk; co-mentor Olga Vasiljeva).
2. Katarina Maher, *The role of cystatins in the innate immune response*: doctoral dissertation, Ljubljana, 2014 (mentor Nataša Kopitar Jerala).
3. Georgy Mikhaylov, *Development of a novel nano-carrier for targeted drug delivery and diagnostics*: doctoral dissertation, Ljubljana, 2014 (mentor Olga Vasiljeva; co-mentor Boris Turk).
4. Vida Puizdar, *Characterization of cathepsin E and its splice variant, and comparison with cathepsin D*: doctoral dissertation, Ljubljana, 2014 (mentor Vito Turk; co-mentor Iztok Dolenc).
5. Ajda Taler-Verčič, *Study of the oligomers of amyloid proteins, using stefin B as a model protein: role in the mechanism of fibril formation and potential function*: doctoral dissertation, Ljubljana, 2014 (mentor Eva Žerovnik).
6. Tilen Vidmar, *Structural characterization of transmembrane protein Trop-2*: doctoral dissertation, Ljubljana, 2014 (mentor Brigita Lenarčič).
7. Matej Vizovišek, *Proteomic approaches for identification of substrates of cysteine proteases*: doctoral dissertation, Ljubljana, 2014 (mentor Boris Turk; co-mentor Marko Fonovič).
8. Anja Kerš, *Caspase-3 cleavage of human autophagins*: master's thesis, Ljubljana, 2014 (mentor Boris Turk).
9. Jaka Košak, *Characterization of the system for drug targeting based on ferriliposomes*: master's thesis, Ljubljana, 2014 (mentor Boris Turk).
10. Aleksander Krajnc, *Biochemical characterization of human cathepsin O*: master's thesis, Ljubljana, 2014 (mentor Brigita Lenarčič).
11. Maja Orešnik, *Expression of recombinant human cathepsin L in yeast *Pichia pastoris* and comparison of its substrate specificity with recombinant mouse cathepsin L*: master's thesis, Ljubljana, 2014 (mentor Boris Turk).

# DEPARTMENT OF MOLECULAR AND BIOMEDICAL SCIENCES

## B-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<sub>2</sub>

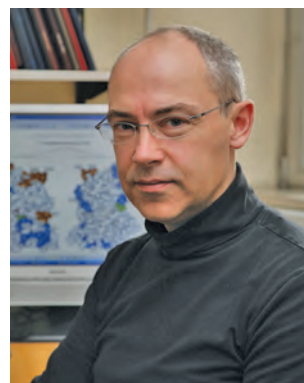
One of the major research topics of the department is secreted phospholipase A<sub>2</sub> (sPLA<sub>2</sub>) originating from animal toxins as well as those found in humans. We are studying the molecular mechanisms of the action of the toxic sPLA<sub>2</sub>, particularly those endowed with presynaptic neurotoxicity, and the role of endogenous sPLA<sub>2</sub> in pathological and physiological processes in mammals.

Along with the development of a new way of renaturing recombinantly expressed sPLA<sub>2</sub> we have endeavoured to produce an enzymatically inactive form of ammodytoxin A (AtxA), a neurotoxic sPLA<sub>2</sub> from the venom of the nose-horned viper (*Vipera ammodytes ammodytes*). We succeeded in this by replacing Asp with Ser at the active site of the AtxA. Analyses with mass spectrometry and the binding properties of the mutant AtxA(D49S) showed that the protein is properly folded. We expect that the use of this molecule will lead to progress in the understanding of the role of phospholipase activity in the neurotoxicity of sPLA<sub>2</sub>, as well as the mechanism of sPLA<sub>2</sub> transport across the plasma membrane and between different cellular compartments. We have already prepared a fluorescently labelled derivative of the AtxA(D49S) mutant and performed preliminary studies on the rat PC12 cell line, which is a model used in our laboratory to study the dynamics of the AtxA cellular uptake, its co-localization with mitochondria and certain intracellular proteins with the use of confocal microscopy. Additionally, we have shown that AtxA binds protein disulphide isomerase in the lumen of the endoplasmic reticulum of PC12 cells also *in vivo* (Figure 1). In a recently prepared paper we suggest that this interaction is important for the translocation of the AtxA from the extracellular space into the cytosol of the cell (J. Oberčkal et al., *PLoS One*, in press). Calmodulin (CaM) is a regulatory protein in the cell cytosol, presumably very important for the intracellular action of AtxA and its mammalian sPLA<sub>2</sub> homologues. In order to dynamically monitor the interaction of the AtxA and CaM in mammalian cells using the FRET method, we have continued with the development of fluorescent derivatives of both proteins.

We set out to identify the sPLA<sub>2</sub> receptor in the presynaptic membrane of motoneurons (N-sPLA<sub>2</sub>R), which plays a crucial role in the neurotoxic effect of these molecules, by using OS<sub>2</sub>, an AtxA-like sPLA<sub>2</sub> from the venom of the coastal taipan (*Oxyuranus scutellatus scutellatus*) since it binds to N-sPLA<sub>2</sub>R with a more than 1000-fold higher affinity than the AtxA. In collaboration with the research group from the Institut de Pharmacologie Moléculaire et Cellulaire, Centre national de la recherche scientifique (CNRS) in Valbonne, France, we continued with the characterization of the photo-reactive derivatives of the recombinant wild-type OS<sub>2</sub> and its chimera with the non-toxic OS<sub>1</sub> from the venom of the same snake, which we will use for the identification of the N-sPLA<sub>2</sub>R.

sPLA<sub>2</sub>s are a physiologically very important family of multifunctional proteins. Their effects do not always depend on their enzymatic activity, but in certain cases also on their binding to other molecules. To discover new sPLA<sub>2</sub> binding molecules we used immuno-affinity chromatography. In the venom of the nose-horned viper we have identified an Atx-binding protein that inhibits the activity of chymotrypsin and belongs to the Kunitz-type protease inhibitors (ChI). Our first results show that the toxicity of the AtxA is higher in the presence of ChI. ChI-like molecules can also be found in mammals. It will be interesting to check their affinity to sPLA<sub>2</sub>s and determine the physiological effects of their interaction with sPLA<sub>2</sub>s (M. Brgles et al., *Anal. Bioanal. Chem.*, 406 (2014), 293–304).

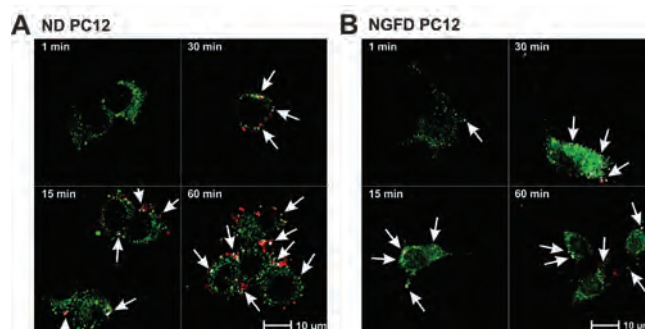
In an attempt to prepare an effective antiserum against the nose-horned viper venom we have discovered that the content of Atx in the venom has a positive correlation with the level of its immunogenicity. A fast and accurate



Head:

**Prof. Igor Krizaj**

**New substances, molecular tools and procedures to improve human and animal health.**



**Figure 1:** Atx and PDI co-localize in living PC12 cells. (A) Non-differentiated (ND) and (B) NGF-differentiated (NGFD) PC12 cells were incubated in the presence of 100 nM <sup>546</sup>Alexa-Atx (red signal) for indicated times. Cells were fixed and protein disulphide isomerase (PDI) stained with anti-PDI antibodies (green signal). The co-localized green and red pixels are shown in white. The arrows point to most extensive areas of co-localization.

method for the determination of Atx content in the venom is therefore one of the crucial steps to develop an effective procedure for the production of a quality antiserum. Together with colleagues from the Technische Universität Vienna, Austria, we have made a step further in the Atx content characterization in the venom by developing an original method, enabling the purification of all three very similar forms of this toxin in only a single step (V. U. Weiss et al., *Electrophoresis*, 35 (2014), 2137–2145).

We were invited to submit a review paper to the *Toxicon* journal (J. Šribar et al., *Toxicon*, 89 (2014), 9–16). A critical overview was presented of all the important research on the action of presynaptically neurotoxic sPLA<sub>2</sub>s reported since our last review in 2007, proposed a hypothesis about the mechanism of action of these toxins and suggested further approaches to test it.

Previous studies have shown that the altered expression of different groups of sPLA<sub>2</sub>s is related to the pathological changes of the different types of cancer, such as cancer of the colon and the rectum, the stomach, the esophagus, the ovary and the prostate. In this respect, it is most likely that either the pro-tumorigenic or anti-tumorigenic role of a certain group of sPLA<sub>2</sub>s depends on the particular type of cancer. Despite the fact that the connection of some mammalian sPLA<sub>2</sub>s with different types of cancer has been recently confirmed, their role in breast cancer is still poorly elucidated. In 2014, we published the results of our in-depth studies where we found that the mRNA expression

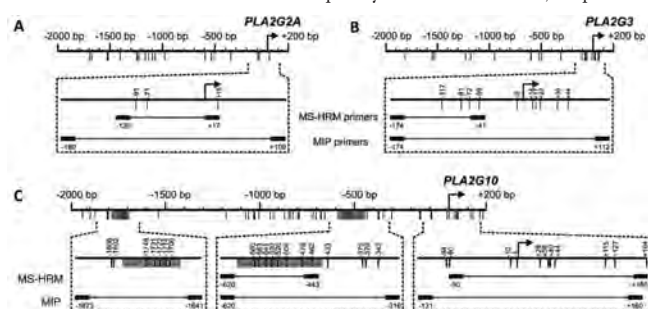


Figure 2: Schematic representation of the promoter gene regions of human group IIA (PLA2G2A), III (PLA2G3) and X (PLA2G10) secreted phospholipases A<sub>2</sub>. The promoter region of each sPLA<sub>2</sub> gene was analysed in an area from 2000 base pairs upstream to 200 base pairs downstream of the putative transcription start site (TSS, indicated by an arrow), revealing two CpG islands (denoted by gray boxes; individual CG doublets are marked by vertical dashes) in the PLA2G10 promoter at the positions around -1700 and -500 relative to the TSS, and none in the promoters of PLA2G2A and PLA2G3. The regions that were analysed by two different methods, MIP (“methylation-independent polymerase chain reaction”) and MS-HRM (“methylation-specific high resolution melting”), and using sequence-specific oligonucleotide primers are shown enlarged. The figure is reproduced from V. Brglez et al., *Biochem. Biophys. Res. Commun.*, 445 (2014), 230–235.

of sPLA<sub>2</sub> groups IIA, III, and X is different both *in vivo*, in tumor biopsies, and *in vitro*, in various cancer cells, from that of the non-cancer cells (V. Brglez et al., *Biochem. Biophys. Res. Commun.*, 445 (2014), 230–235). We have found that one of the main causes for the observed differences in the expression of sPLA<sub>2</sub>s is the modified epigenetic regulation of their gene expression in breast-cancer cells. The expression of sPLA<sub>2</sub>s is thus differentially regulated by DNA methylation and histone acetylation, where appropriate (*i.e.*, their) genes are most highly silenced in the aggressive, triple-negative breast-cancer cells, MDA-MB-231, due to the combined action of both mechanisms. The transcription start site promoter region and the upstream CpG islands (Figure 2), exclusive to the group X sPLA<sub>2</sub> gene, have variable roles in the regulation of the sPLA<sub>2</sub> expression. Recently, in 2013, we also found that exogenously added human sPLA<sub>2</sub>-X, but not sPLA<sub>2</sub>-IIA, induced lipid droplet formation, particularly in the highly tumorigenic MDA-MB-231 cells in an enzymatic activity-dependent manner, thereby stimulating cell proliferation and significantly prolonging cell survival under serum (nutrient) deprivation-induced stress. The results also suggested that free fatty acids, in particular oleic acid, released from membrane phospholipids by the enzymatic action of sPLA<sub>2</sub>-X, are primarily responsible for these effects. In accordance with these findings, the pro-tumorigenic effect of sPLA<sub>2</sub>-X was particularly evident in the increased survival (viability) of highly tumorigenic cells, but not of that of non-tumorigenic and weakly tumorigenic breast-cancer cells. Our latest research, published in 2014, thus convincingly shows that the differential

expression of human sPLA<sub>2</sub>-IIA, -III and -X in breast-cancer cells is due to the different level of epigenetic silencing, both by hypermethylation of genomic DNA and deacetylation of histone proteins, of particular phospholipase genes.

Together with the Institute of Biochemistry, Faculty of Medicine, University of Ljubljana, we participated in a study on the role of human sPLA<sub>2</sub>-IIA in ovarian endometriosis. The latter is a heterogeneous progressive disease, with the presence of endometrioma (cysts) in the ovaries. It is a leading cause of chronic pelvic pain and subfertility, and it can affect up to ten percent of the women of reproductive age. The availability of less-invasive and timely diagnostic methods for women with endometriosis would thus be highly beneficial. Previous research by colleagues from the Faculty of Medicine has also indicated that sPLA<sub>2</sub>-IIA could serve as a potential biomarker for ovarian endometriosis. One-hundred and sixteen women, 70 among them with ovarian endometriosis, were included in the investigation that was published online last year (V. Kocbek et al., *Gynecol. Endocrinol.*, in press). In the cases of ovarian endometriosis, we observed a significant increase in the synthesis of sPLA<sub>2</sub>-IIA mRNA in cancer tissue (endometrioma) compared with normal endometrium, but not the higher concentration of the sPLA<sub>2</sub>-IIA protein in the peritoneal fluid and serum. The results obtained show that the sPLA<sub>2</sub>-IIA is involved in pathophysiological changes in the ovarian endometriosis, but it is not useful as a diagnostic biomarker for this disease.

Based on our renowned research of the (patho)physiological role of sPLA<sub>2</sub>s, we have been invited to prepare a review on the different operating modes of sPLA<sub>2</sub>s in cancer, which was published in the past year (V. Brglez et al., *Biochimie*, 107 (2014), 114–123). Mostly it reflects the action of the already-mentioned three groups of sPLA<sub>2</sub>s, whose altered expression has been observed in several cancer types both in mouse models and in patients, *i.e.*, IIA, III and X. It is becoming increasingly clear that the involvement of sPLA<sub>2</sub>s in various types of cancer includes several

modes of operation of these membrane-active phospholipase enzymes, depending on a particular cell environment. Firstly, already some time ago, the role of sPLA<sub>2</sub>s in cancer has been connected with their enzyme activity and the consequent release of free fatty acids, *i.e.*, basic building blocks in the synthesis of an array of biologically active lipid mediators, particularly the products of arachidonic acid, called eicosanoids that promote tumorigenesis by inhibiting cell death (apoptosis), increasing local inflammation and the formation of new blood vessels (angiogenesis). Secondly, many of the biological effects are independent of the enzyme (phospholipase) activity and indicate an additional role of receptors in the action of sPLA<sub>2</sub>s in the development of cancer. And thirdly, the latest research, of which a large proportion was carried out by our group, discovered a very important role of sPLA<sub>2</sub>s in the regulation of basic lipid metabolism (lipid droplet formation and lipid degradation in the mitochondria), which may affect various physiological and pathological cellular changes, including the formation and development of cancer.

The activity of our group in the field of sPLA<sub>2</sub> is evidently well known, also to the editors of the *Protein and Peptide Letters*, as they invited us to prepare a review article on the role of these molecules in the mammalian immune system (I. Križaj, *Protein Pept. Lett.*, 21 (2014), 1201–1208).

### Other pharmacologically active components from natural toxins

In 2014 we continued to systematically analyse the components of the nose-horned viper that affect the blood-coagulation process, *i.e.*, haemostasis (Figure 3). We succeeded to publish a description of heterodimeric haemorrhagic metalloproteinase, VaH4 (A. Leonardi et al., *Toxicon*, 77 (2014), 141–155).

Upon the editor's invitation we prepared a review paper describing our research on haemostatically active components from the venom of the nose-horned viper (T. Sajevec et al., *Toxin Rev.*, 33 (2014), 33–36). With our colleagues from the Imunološki zavod Zagreb, Croatia, and Technische Universität Vienna, Austria, we described another very interesting molecule from the venom of this snake. The serine proteinase VaSP1 with an unconventional structure of the active site, according to its substrate specificity and the fact that it prolongs the prothrombin and the activated partial thromboplastin time, very likely possesses an anticoagulant effect (T. Kurtović et al., *Toxicon*, 77 (2014), 93–104).

In 2014, two additional interesting groups of molecules from the venom of the nose-horned viper were a focus of our research, *i.e.*, disintegrins and CRISPs (Cysteine Rich Secretory Proteins). Disintegrins are polypeptides that bind to integrin molecules and thus impair their function. CRISPs are toxic and they block ion channels in different cells, causing, for example, the paralysis of peripheral smooth muscles and hypothermia. CRISPs and disintegrins from the venom of the nose-horned viper were purified and biochemically characterized, while the research on their pathophysiological effects is still being conducted.

### High-throughput genetics and functional genomics in yeast *Saccharomyces cerevisiae*

In the field of genetics, in recent years we have seen a rapid development in techniques and methods for polygenic traits analyses, which have been spurred by recent developments in genomics. Our group started coordinating a European consortium whose aim is to combine these methods with metabolic engineering and synthetic biology tools, in order to develop complex cell factories that in the future will play a very important role in the development of the bioeconomy (<https://krog.sta.si/2079947>).

Inter-organelle communication is a rapidly developing subfield of cell biology that plays a crucial role for the system-wide understanding of cells. In 2014 we finalized a study in which we discovered a new way of interaction between mitochondria and peroxisomes. This discovery could have an important impact on the design of biotechnological processes for lipid-based bioproducts production, and on the understanding of the development of metabolic syndrome in humans.

Our colleague from the department, currently a postdoc at the University of Toronto, participated in the development of a new method to analyse protein-protein interactions, the mammalian-membrane two-hybrid assay (J. Petschnigg et al., *Nat. Methods*, 11 (2014), 585–592).

In 2014 we took over the organization of the ISSY31 conference – International Specialised Symposium on Yeast, which gathered 250 world-leading researchers from the field of yeast fermentations (Figure 4). We also co-organized an international workshop on functional genomics (<http://biolab.github.io/functional-genomics-workshop/>), which attracted over 50 PhD students and post-doctoral fellows from Slovenia and abroad.

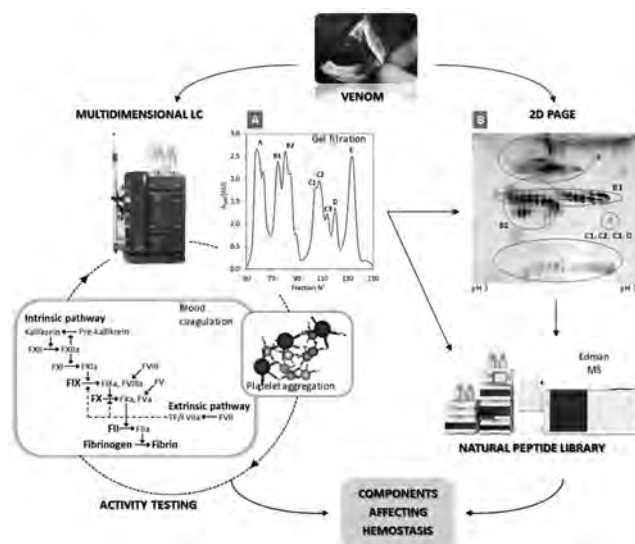


Figure 3: Proteomic analysis of haemostatically active components in the nose-horned viper venom. (A) Initial fractionation of the venom proceeded on Sephacryl S-200. (B) 2D PAGE analysis of the crude venom. Groups of proteins found in particular size-exclusion chromatography fraction (A) are encircled. The figure is reproduced from T. Sajevec et al., *Toxin Rev.*, 33 (2014), 33–36.





Figure 4: 31<sup>st</sup> International Specialised Symposium on Yeast, covering all the aspects of yeast fermentations, took place in the Vipava valley in October 2014. The conference was co-organized by our department with Prof. Uroš Petrovič as the executive chairman of the organizing committee.

Neonicotinoid insecticides were rather notorious in 2013 because of their proposed toxicity for bees and other non-target organisms, on the basis of which they were banned in the EU from April 2013. Using chemogenomics analysis in the yeast model we have determined the side effects of neonicotinoid insecticides, and especially of additives from insecticide formulations. We have shown examples where additives are even more toxic than neonicotinoids themselves (M. Mattiazzi Ušaj et al., *Chemosphere*, 104 (2014), 91–96).

#### Pathogenomics of novel virulence factors

The ability of pathogenic bacteria to cause disease in a susceptible host is determined by multiple virulence factors acting individually or together at different stages of the infection. Discovering the virulence factors of pathogenic bacteria is a key to understanding pathogenesis and for the identification of targets for novel drugs and the design of new vaccines. Recently, we have found that eukaryotic cystatins and stefins have been acquired and co-opted by a few bacteria (Figure 5). Bacterial cystatins and stefins could play an important role in self-defence or attack against host inflammatory and immune responses, by inhibiting cysteine cathepsins that are essential

for host innate and acquired immunity. Our hypothesis is that some pathogenic bacteria have evolved independently a novel anti-immune strategy by horizontal gene transfer (similarly as eukaryotic parasites) to overcome host innate immunity. In order to demonstrate the biochemical activity of bacterial stefins, we expressed *Vibrio cholerae* stefin (VCA0935) and *Bacteroides fragilis* fusion inhibitor containing chagasin and cystatin domains (BF1388). We explored the inhibitory properties of recombinant proteins VCA0935 and BF1388 and determined their interaction constants with diverse cysteine proteases, cathepsins L, S, K, V, B and papain. Both VCA0935 and BF1388 were found to act as fast and tight binding inhibitors of endopeptidases cathepsins K, S, V, L and papain; however, their interaction with exopeptidase cathepsin B was several orders of magnitude weaker. Interestingly, the bacterial stefins inhibit the endopeptidase activity of cathepsins S, K, L and V, which are all important players in the host adaptive and innate immunity. There are a very few cases where protease inhibitors have been shown to assist pathogens in invading the eukaryotic hosts by inhibiting host proteases. Stefins and cystatins with inhibitory spectra for the papain family of cysteine proteases are especially suited to inhibit the numerous eukaryotic host cysteine proteases during infection. In this way, the bacterial stefins and cystatins could function in the invasion and dissemination of the pathogens.

The expert body of the Scientific Council at the Slovenian Research Agency selected our work, in which we traced the genesis and evolution of retroelement-derived multigene families of domesticated genes (J. Kokošar in D. Kordiš, *Mol. Biol. Evol.*, 30 (2013), 1015–1031), as the most important scientific achievement of 2013 in the field of Biochemistry and Molecular Biology.

#### Other subjects

In 2014 we also worked on several projects out of the thematic scope of our department.

We collaborated intensively with the colleagues from the Department of Biology, the Biotechnical Faculty, University of Ljubljana, at elucidating the haemolytic activity of bovine erythrocytes with an ethanol extract of the *Aspergillus niger* mycelium (M. Novak et al., *Molecules*, 19 (2014), 9051–9069).

With colleagues from the Department of Biochemistry, Molecular and Structural Biology at the Jožef Stefan Institute we contributed to an understanding of the role of human stefin B in cellular response to protein aggregates with autophagy, by expressing it in *Saccharomyces cerevisiae* and identifying its genetic interactions (M. Polajnar et al., *PLoS One*, 9 (2014), e102500).

In collaboration with our colleagues, rheumatologists from the University Medical Centre Ljubljana, we improved the isolation procedure for two human serum proteins that are essential for the diagnostics of the anti-phospholipid syndrome (A. Artnjak et al., *J. Immunol. Res.*, 2014 (2014), e195687).

With our colleagues from the Institute of Biochemistry, Medical Faculty, University of Ljubljana, we collaborated on the discovery of new substances with antifungal activity with tri-dimensional modelling of the structure and mapping of the active site of proteins from the family of fungal cytochrome P450 monooxygenases (P. Jawallapersand et al., *PLoS One*, 9 (2014), e107209).

## Some outstanding publications in the past year

1. Šribar, J. Oberčkal, J. and Križaj, I.: Understanding the molecular mechanism underlying the presynaptic toxicity of secreted phospholipases A<sub>2</sub> – an update. *Toxicon*, 89 (2014), 9–16
2. Brglez, V., Pucer, A., Pungerčar, J., Lambeau, G. and Petan, T.: Secreted phospholipases A<sub>2</sub> are differentially expressed and epigenetically silenced in human breast cancer cells. *Biochem. Biophys. Res. Commun.*, 445 (2014), 230–235
3. Brglez, V., Lambeau, G. and Petan, T.: Secreted phospholipases A<sub>2</sub> in cancer: Diverse mechanisms of action. *Biochimie*, 107 (2014), 114–123
4. Leonardi, A., Sajevec, T., Kovačič, L., Pungerčar, J., Lang Balija, M., Halassy, B., Trampuš-Bakija, A. and Križaj, I.: Hemorrhagin VaH4, a covalent heterodimeric P-III metalloproteinase from *Vipera ammodytes ammodytes* with potential anti-tumour activity. *Toxicon*, 77 (2014), 141–155
5. Petschnigg, J., Groisman, B., Kotlyar, M., Taipale, M., Zheng, Y., Kurat, C. F., Sayad, A., Sierra, J. R., Mattiazzi Usaj, M., Snider, J., Nachman, A., Krykbaeva, I., Tsao, M.-S., Moffat, J., Pawson, T., Lindquist, S., Jurisica, I. and Stajljar, I.: The mammalian-membrane two-hybrid assay (MaMTH) for probing membrane-protein interactions in human cells. *Nat. Methods*, 11 (2014), 585–592

## Awards and Appointments

1. Janez Kokošar, Dušan Kordiš: Award of the Slovenian Research Agency for an exceptional scientific achievement in 2013 in Slovenia in the field of Biochemistry and Molecular Biology, Genesis and regulatory wiring of retroelement-derived domesticated genes

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## INTERNATIONAL PROJECT

1. 7FP - YeSVitE; Yeasts for the Sustainability in Viticulture and Oneology  
Prof. Uroš Petrovič  
European Commission

## RESEARCH PROGRAM

1. Toxins and Biomembranes  
Prof. Igor Križaj

## R & D GRANTS AND CONTRACTS

1. Apoptotic Effects of Alkylpyridinium Compounds on Lung Adenocarcinoma Cells  
Prof. Igor Križaj
2. Molecular Description of Lipid Membrane Changes in Disease  
Prof. Igor Križaj
3. Thermophoretic Guidance, Accumulation and Sorting of Biomolecules in Microfluidic Devices  
Prof. Igor Križaj
4. Discovering Innovative Drugs for Regulation of Haemostasis by Venomics of the *Vipera ammodytes ammodytes* Snake  
Prof. Igor Križaj
5. Pathogenomics and Systems Biology of New Virulence Factors in Pathogenic Bacteria  
Prof. Dušan Kordiš
6. Definition of Molecular Parameters for Protection of Carniolan Honeybee  
Prof. Igor Križaj

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## VISITORS FROM ABROAD

1. Prof. Angelica Ganga, Universidad de Santiago de Chile, Chile, 3 January–8 February 2014
2. Sofia Dashko, Wine Research Centre, University of Nova Gorica, Nova Gorica, 27 January–28 March 2014
3. Dr. Gerard Lambeau, Institute de Pharmacologie Moleculaire et Cellulaire, Universite Nice, Sophia Antipolis, Francija, 18–20 October 2014

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## STAFF

### Researchers

1. Prof. Dušan Kordiš
2. Prof. Igor Križaj, Head
3. Dr. Adrijana Leonardi
4. Prof. Uroš Petrovič
5. Prof. Jože Pungerčar

### Postdoctoral associates

6. Dr. Janez Kokošar, left 01. 02. 14
7. Dr. Mojca Mattiazzi Ušaj
8. Asst. Prof. Toni Petan

9. Dr. Jernej Šribar

### Postgraduates

10. Dr. Vesna Brglez, left 01. 10. 14
11. Minca Klobčar, B. Sc.
12. Jernej Oberčkal, B. Sc., left 01. 05. 14

### Technical officer

13. Mojca Brložnik, B. Sc.

### Technical and administrative staff

14. Igor Koprivec
15. Darja Žunič Kotar

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## ORIGINAL ARTICLE

1. Andrej Artenjak, Adrijana Leonardi, Igor Križaj, Aleš Ambrožič, Snežna Sodin-Semrl, Borut Božič, Saša Čučnik, "Optimization of unnicked  $\beta$ -glycoprotein I and high avidity anti- $\beta$ -glycoprotein I antibodies isolation", *J. immunol. res.*, vol. 2014, pp. 195687-1-195687-8, 2014.
2. Marija Brgles, Tihana Kurtović, Lidija Kovačič, Igor Križaj, Miloš Barut, Maja Lang Balija, Günter Allmaier, Martina Marchetti Deschmann, Beata Halassy, "Identification of proteins interacting with ammodytoxins in *Vipera ammodytes ammodytes* venom by immunofluorescence and immunoprecipitation", *Anal. bioanal. chem.*, vol. 406, no. 1, pp. 293-304, 2014.
3. Vesna Brglez, Anja Pucer Janež, Jože Pungerčar, Gérard Lambeau, Toni Petan, "Secreted phospholipases  $A_2$  are differentially expressed and epigenetically silenced in human breast cancer cells", *Biochem. biophys. res. commun.*, vol. 445, no. 1, pp. 230-235, 2014.
4. Poojah Jawallapersand, Samson Sitheni Mashele, Lidija Kovačič, Jure Stojan, Radovan Komel, Suresh P. Babu, Nada Kraševc, Khajamohiddin Syed, "Cytochrome P450 monooxygenase CYP53 family in fungi: comparative structural and evolutionary analysis and its role as a common alternative anti-fungal drug target", *PLoS one*, vol. 9, iss. 9, pp. 1-15, e107209, Sep. 2014.
5. Tihana Kurtović, Marija Brgles, Adrijana Leonardi, Maja Lang Balija, Tamara Sajevec, Igor Križaj, Günter Allmaier, Martina Marchetti Deschmann, Beata Halassy, "VaSP1, catalytically active serine proteinase from *Vipera ammodytes ammodytes* venom with unconventional active site triad", *Toxicon (Oxford)*, vol. 77, pp. 93-104, 2014.
6. Adrijana Leonardi, Tamara Sajevec, Lidija Kovačič, Jože Pungerčar, Maja Lang Balija, Beata Halassy, Alenka Trampuš-Bakija, Igor Križaj, "Hemorrhagin VaH4, a covalent heterodimeric P-III metalloproteinase from *Vipera ammodytes ammodytes* with a potential antitumor activity", *Toxicon (Oxford)*, vol. 77, pp. 141-155, 2014.
7. Mojca Mattiazzi, Petra Kaferle, Alenka Toplak, Polonca Trebše, Uroš Petrovič, "Determination of toxicity of neonicotinoids on the genome level using chemogenomics in yeast", *Chemosphere (Oxford)*, vol. 104, pp. 91-96, 2014.
8. Maruša Novak, Kristina Sepčič, Nada Kraševc, Igor Križaj, Peter Maček, Gregor Anderluh, Graziano Guella, Ines Mancini, "Targeted lipid analysis of haemolytic mycelial extracts of *Aspergillus niger*", *Molecules (Basel)*, vol. 19, no. 7, pp. 9051-9069, 2014.
9. Julia Petschnigg *et al.* (18 authors), "The mammalian-membrane two-hybrid assay (MaMTH) for probing membrane-protein interactions in human cells", *Nature methods*, vol. 11, no. 5, pp. 585-592, 2014.
10. Mira Polajnar, Tina Zavašnik-Bergant, Katja Škerget, Matej Vizovišek, Robert Vidmar, Marko Fonović, Nataša Kopitar-Jerala, Uroš Petrovič, Susanna Navarro, Salvador Ventura, Eva Žerovnik, "Human stefin B role in cell's response to misfolded proteins and autophagy", *PLoS one*, vol. 9, no. 7, pp. e102500-1-e102500-15, 2014.
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neurotoxic phospholipases  $A_2$  of *Vipera ammodytes ammodytes* venom", *Electrophoresis*, vol. 35, issue 15, pp. 2137-2145, 2014.

## REVIEW ARTICLE

1. Khadija Mohamed Ahmad, Janez Kokošar, Xiaoxian Guo, Zhenglong Gu, Olena P. Ishchuk, Jure Piškur, "Genome structure and dynamics of the yeast pathogen *Candida glabrata*", *FEMS yeast research*, vol. 14, no. 4, pp. 529-535, 2014.
2. Vesna Brglez, Gérard Lambeau, Toni Petan, "Secreted phospholipases  $A_2$  in cancer", *Biochimie (Paris)*, vol. 107, part A, pp. 114-123.
3. Igor Križaj, "Roles of secreted phospholipases  $A_2$  in the mammalian immune system", *Prot. peptide letters*, vol. 21, no. 12, str. 1201-1208.
4. Jernej Šribar, Jernej Oberčkal, Igor Križaj, "Understanding the molecular mechanism underlying the presynaptic toxicity of secreted phospholipases  $A_2$ : an update", *Toxicon (Oxford)*, vol. 89, pp. 9-16, 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Nuša Kapušin, Uroš Petrovič, Daša Jevšinek Skok, Minja Zorc, Tanja Kunej, Simon Horvat, "Bioinformatična analiza evolucijske ohranjenosti genov, udeleženih v metabozmu maščob", In: *iTIME brainstorming: zbornik prispevkov = proceedings*, 2. Simpozij raziskovalne mreže Integratomics TIME Domžale, 19. 12. 2013, Tanja Kunej, ed., Jana Obšteter, ed., Daša Jevšinek Skok, ed., Domžale, Univerza v Ljubljani, Biotehniška fakulteta, Oddelek za zootehniko, 2014, pp. 2-6.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Birgit Ploier, Günther Daum, Uroš Petrovič, "Molecular mechanisms in yeast carbon metabolism: lipid metabolism and lipidomics", In: *Molecular mechanisms in yeast carbon metabolism*, Jure Piškur, ed., Heidelberg [etc.], Springer, cop. 2014, pp. 169-215.

## UNIVERSITY, HIGHER EDUCATION OR HIGHER VOCATIONAL EDUCATION TEXTBOOK

1. Nataša Debeljak, Simon Horvat, Peter Juvan, Tanja Kunej, Uroš Petrovič, Tadeja Režen, *Funkcijska genomika: praktikum*, 1. izd., Ljubljana, Medicinska fakulteta, 2014.

## MENTORING

1. Vesna Brglez, *Regulation and action of secreted phospholipases  $A_2$  in breast cancer*: doctoral dissertation, Ljubljana, 2014 (mentor Jože Pungerčar; co-mentor Toni Petan).
2. Anja Pucer, *Role of secretory phospholipases  $A_2$  in breast cancer*: doctoral dissertation, Ljubljana, 2014 (mentor Jože Pungerčar; co-mentor Toni Petan).
3. Tamara Sajevec, *Hemostatically-active proteins from *Vipera a. ammodytes* venom*: doctoral dissertation, Ljubljana, 2014 (mentor Igor Križaj).

# DEPARTMENT OF BIOTECHNOLOGY

## B-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 of 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 on the search for new biotechnological approaches and products.*



Head:  
**Prof. Janko Kos**

In 2014 in the field of research on fungal protease inhibitors we focused on a precise analysis of the inhibitory mechanism of cnispin from clouded agaric and cospin from the inky cap, both trypsin-specific inhibitors. The analysis revealed the exceptional versatility of fungal protease inhibitors with a beta-trefoil fold, as it showed that the loop  $\beta 11$ - $\beta 12$  is recruited for the trypsin inhibitor in cnispin, which distinguishes cnispin from all other known beta-trefoil fold trypsin inhibitors. Similar inhibitors from plants and fungi utilize other loops for protease inhibition where the same protease can be inhibited through different loops and the inhibition of different proteases can be achieved through the same loop. Furthermore, we have shown the insecticidal activity of clitocyprin, the cysteine protease inhibitor from clouded agaric, against Colorado potato beetle larvae. Like we have previously shown for cysteine protease inhibitors from parasol mushroom, macrocypins, clitocyprin also inhibits digestive cysteine proteases, intestains, and it does not elicit the adaptive response in larval guts. This establishes mushrooms as an attractive source of novel biopesticides.

A study in cooperation with the National Institute of Biology on novel antibacterial compounds from mushrooms using the plant pathogenic bacterium *Ralstonia solanacearum* as the model led to the isolation and characterization of a protein complex with L-amino acid oxidase activity. We developed a new method for the in-gel detection of the L-amino acid oxidase activity.

The studies in the field of glycobiology in 2014 focused on lectins from different mushrooms and their effects on different cell lines with an emphasis on immune cells. Furthermore, we are developing these lectins as tools for targeted delivery. Additionally, we have performed an applicative project in the field of lectin research for an industrial partner.

The continuing study on the involvement of proteases in plant response to drought showed that in the model resurrection plant *Ramonda serbica* there are amino- and endo-peptidases, the activities of which are much greater in dehydrated compared to hydrated leaves, indicating their involvement in the recovery of vegetative tissue from complete desiccation.

The studies on the role of proteolytic enzymes in physiological and pathological conditions were focused on the regulation of the action of cytotoxic cells. In this process the role of lysosomal enzymes cathepsins C and H is crucial since they are the major convertases in the processing of progranzyms into active forms, which trigger apoptosis in target cells. Cathepsins C and H are controlled in secretory vesicles by the endogenous inhibitor cystatin F. Cystatin F is translocated to vesicles as an inactive dimer, which monomerizes after the proteolytic cleavage of the N terminal peptide and becoming an active inhibitor of cathepsins C and H. In the year 2014 we developed several mutants of cystatin F, which will enable us a to discover precise mechanism of action of cystatin F in cytotoxic cells. Using recently developed methods of gene editing involving RNA-guided endonuclease (RGEN) technology, also referred to as a Clustered,

- **Cathepsin X is an important tumour promotor**
- **Mutant TDP-43 in neural stem cells derived from induced pluripotent stem cells is significantly reduced.**
- **Insecticidal activity of clitocyprin, the cysteine protease inhibitor from clouded agaric, against Colorado potato beetle larvae was demonstrated.**

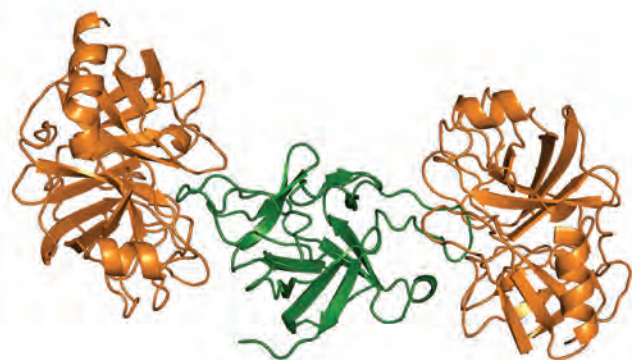


Figure 1: A model of cospin (green) in a complex with two trypsins (orange).

- **Surface display on *Lactococcus lactis* enables the preparation of non-recombinant (non-GMO) organisms, which opens up numerous possibilities for therapeutic and food application.**
- **A new method for the in-gel detection of L-amino acid oxidase activity was developed.**
- **42 scientific papers in journals with an impact factor were published in 2014. A US patent was granted, and an international patent application was also filed.**





Figure 2: Fly agaric, a source of bioactive compounds.

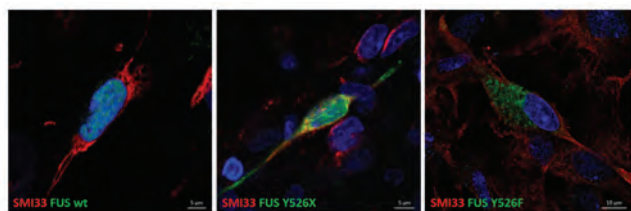


Figure 3: Co-culture of electroporated rat embryonic spinal cord explants and human primary muscle cells. The explants were electroporated with pEGFP constructs carrying FUS wt, FUS Y526X or FUS Y526F (green). Neurites are marked by SMI33 (red).

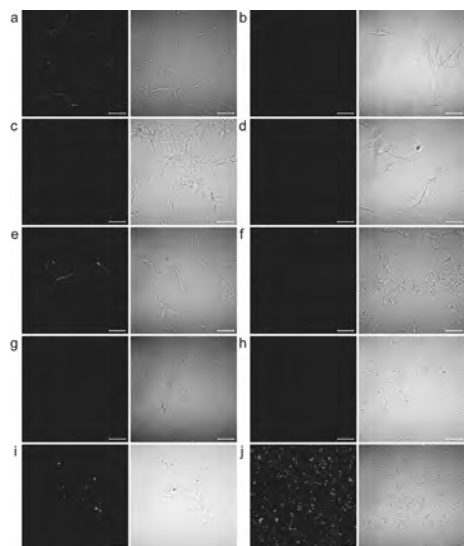


Figure 4: Fluorescence microscopy of *Lactobacillus* sp. cells after incubation with DARPin I07-cA fusion protein-containing medium and detection with FITC-conjugated human IgG. A: *Lb. acidophilus*; b: *Lb. delbrueckii* ssp. *bulgaricus*; c: *Lb. casei*; d: *Lb. gasseri* ATCC33323; e: *Lb. gasseri* K7; f: *Lb. paracasei*; g: *Lb. reuteri*; h: *Lb. plantarum*; i: *Lb. rhamnosus*; j: *Lb. salivarius*. Left: Fluorescence image. Right: Bright field image. Bar = 20  $\mu$ m. Superior binding to the surface of *Lb. salivarius* can be observed.

Regularly Interspaced Palindromic Repeat Associated Proteins (CRISPR/Cas) system, we silenced the expression of cystatin F in cytotoxic cells and confirmed its active role in the regulation of cytotoxicity. Using the same method we also overexpressed cystatin F in mammalian cells. To determine direct interactions between the molecules of the proteolytic system in cytotoxic cells, the proximity ligation method (PLA) was introduced, giving us information about protein interactions in particular cell compartments.

In the field of molecular neurobiology, we published several research studies in reputable journals on the molecular processes underlying frontotemporal dementia (FTD) and amyotrophic lateral sclerosis (ALS). In two papers we published the results on the involvement of TDP-43 in the disease. We looked at the differential roles of the ubiquitin proteasome system (UPS) and autophagy in the clearance of soluble and aggregated TDP-43 species (Scotter et al., Journal of Cell Science). In the second paper (Nishimura et al., PLOS One) we looked for ways of reducing the mutant TDP-43 load with allele-specific knockdown. We showed the reduction of the mutant TDP-43 in neural stem cells derived from induced pluripotent stem cells. Also, we presented that the GGGGCC stretches of DNA that are involved in C9orf72 associated ALS and FTLD can form special secondary structures called G-quadruplexes (Šket et al., Neurobiology of Ageing). Of the review papers we would highlight the invited commentary by the leading journal Brain (Lee et al., Brain) discussing the importance and implications of reported miRNA expression changes in the serum of ALS patients.

In the field of lactic acid bacteria, we continued with the improvements of surface display on *Lactococcus lactis* and bacteria from the genus *Lactobacillus*. Surface binding was achieved with LysM repeats, which enable the binding to peptidoglycan. LysM repeats were assembled into fusion proteins with two model binding proteins from the group of DARPins. The latter were successfully displayed on the surface of most of the bacteria tested. Fusion proteins were expressed in *Lactococcus lactis* and directed into the growth medium, which served, after the removal of producer cells, as a source of fusion proteins. The expressed fusion proteins were bound to the surface of 10 species of bacteria from the genus *Lactobacillus*. The strongest binding was observed with *Lactobacillus salivarius* ATCC 11741, which is probably due to its exceptional surface properties. The surface display was additionally improved by the addition of sublethal concentrations of antibiotics erythromycin and chloramphenicol to the growth medium. This type of surface display enables the preparation of non-recombinant (non-GMO) organisms, which opens up numerous possibilities for therapeutic and food application, particularly with the use of DARPins against custom targets.

In 2014 we were granted the US Patent US 8754198 for related technology, which enables the presentation of a TNF $\alpha$ -binding molecule on the surface of *Lactococcus lactis*. The technology represents a potential alternative for the treatment of inflammatory bowel disease, permitting a patient-friendlier administration and direct action at the site of inflammation in the gastrointestinal tract. The technology of TNF $\alpha$ -binding was upgraded with a heterologous surface display on non-genetically modified bacteria. An efficient display on the surface of *Lactobacillus salivarius* ATCC 11741 was established.

The results of the research work at the Department of Biotechnology in 2014 were published in 42 scientific papers in journals with an impact factor. In 2014 we received, as principal investigators, three ARRS grants and two additional grants for young investigators (Ph.D. students). We also received two international bilateral grants. The Ph. D. student Simona Darovic received a fellowship from Ad futura for eight months research work at King's College, London, where she investigated the impact of post-translational modifications on the cell localisation of proteins, associated with ALS (Figure 3). The student Gašper Žun from Gimnazija Kranj received a Golden Award in the field of Biology at the 48<sup>th</sup> National Meeting of Young Researchers 2014 organized by the Association for Technical Culture of Slovenia for the high school student research work done at our department. The members of the department co-organized several scientific meetings and were also very active in pedagogical work as lecturers and mentors to students preparing diploma and doctoral theses at universities in Slovenia and abroad.

## Some outstanding publications in the past year

1. Kos, J., Vižin, T., Pečar Fonović, U., Pišlar, A., et al.: Intracellular signaling by cathepsin X: molecular mechanisms and diagnostic and therapeutic opportunities in cancer. *Seminars in cancer biology*, ISSN 1044-579X, 2014, doi: 10.1016/j.semcancer.2014.05.001., IF 9,1.
2. Lee, Youn-Bok, Rogelj, B., Shaw, C. E.: A serum microRNA signature for amyotrophic lateral sclerosis reveals convergent RNA processing defects and identifies presymptomatic mutation carriers. *Brain*, ISSN 0006-8950, 2014, vol. 137, no. 11, str. 2875-2876, IF 10,2.
3. Šket, P., Pohleven, J., Kovanda, A., Štalekar, M., Župunski, V., Zalar, M., Plavec, J., Rogelj, B.: Characterization of DNA G-quadruplex species forming from C9orf72 G<sub>4</sub>C<sub>2</sub> expanded repeats associated with amyotrophic lateral sclerosis and frontotemporal lobar degeneration. *Neurobiology of aging*, ISSN 0197-4580, 2014, 21 str., doi: 10.1016/j.neurobiolaging.2014.09.012, IF 4,9.

## Patent granted

1. Mojca Lunder, Matjaž Ravnikar, Borut Štrukelj, Aleš Berlec, Boris Čeh, Modified food grade microorganism for treatment of inflammatory bowel disease, US8754198 (B2), United State Patent Office, 17.6.2014.

## INTERNATIONAL PROJECTS

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. The Role of Cysteine Proteases and their Inhibitors in Split Energy of Natural Killer Cells to Tumor Cells<br/>Prof. Janko Kos<br/>Slovenian Research Agency</li> <li>2. Mechanism of C9orf72 Extended Repeat Pathogenicity in ALS and FTD<br/>Prof. Boris Rogelj<br/>Slovenian Research Agency</li> <li>3. Disrupted RNA Processing in Amyotrophic Lateral Sclerosis<br/>Prof. Boris Rogelj<br/>Slovenian Research Agency</li> </ol> | <ol style="list-style-type: none"> <li>4. Genetics and Pharmacogenomics of Inflammatory Bowel Diseases and Genetically Related Chronic Immune Diseases<br/>Prof. Boris Rogelj</li> <li>5. Pathogenic Mechanism of the C9orf72 Expanded Hexanucleotide Repeat Mutation in Neurodegeneration<br/>Prof. Boris Rogelj</li> <li>6. Inhibitors of Cysteine Carboxypeptidases as Regulators of Autoimmune and Neurodegenerative Processes<br/>Prof. Janko Kos</li> <li>7. Response to Water Stress in Common Bean (<i>Phaseolus vulgaris</i> L.): Proteomic Analysis and QTL Mapping<br/>Prof. Janko Kos</li> <li>8. Nitroxoline and its Derivatives as New Antitumour Drugs<br/>Dr. Jerica Sabotič</li> <li>9. The Role of Cysteine Protease Inhibitors in NK Cell Mediated Lysis of Tumour Cells<br/>Prof. Janko Kos</li> <li>10. Post-Transcriptional Regulatory Networks in Neurodegenerative Diseases<br/>Prof. Boris Rogelj</li> </ol> |
|---|---|

## RESEARCH PROGRAM

1. Pharmaceutical Biotechnology: Knowledge for Health  
Prof. Janko Kos

## R & D GRANTS AND CONTRACTS

1. Protein Engineering of Recombinant Probiotic Lactic Acid Bacteria for Treatment of Irritative Bowel Disease  
Prof. Borut Štrukelj
2. Transport and RNA Binding of TDP-43 and FUS - Implications for ALS/FTLD Spectrum of Neurodegenerative Disease  
Prof. Boris Rogelj
3. Dysregulation of TDP-43 Expression in Amyotrophic Lateral Sclerosis and Frontotemporal Lobar Degeneration  
Prof. Boris Rogelj

## NEW CONTRACTS

1. Development and Application of New Methods of Genetic Engineering of Probiotic Lactic Acid Bacteria  
Asst. Prof. Aleš Berlec  
Labena d. o. o.
2. Cooperation in the Area of Implementation of Bioprocess Technology for Use in Development of Biomedicines and Implementation of Mechanical Models for Protein Isolation Procedures  
Dr. Jerica Sabotič  
Lek d. d.

## STAFF

### Researchers

1. Prof. Kristina Gruden\*
2. **Prof. Janko Kos\***, Head
3. Prof. Boris Rogelj
4. Prof. Borut Štrukelj\*

### Postdoctoral associates

5. Asst. Prof. Aleš Berlec
6. Dr. Maruška Budič
7. Dr. Anja Kovanda
8. Dr. Milica Perišić Nanut
9. Dr. Jure Pohleven
10. Dr. Sonja Prpar Mihevc
11. Dr. Anja Pucer Janež
12. *Dr. Katja Rebolj, left 01. 03. 14*

13. Dr. Jerica Sabotič
14. *Dr. Sabina Vatovec, left 01. 07. 14*

### Postgraduates

15. Ana Bajc Česnik, B. Sc.
16. Simona Darovic, B. Sc.
17. Mateja Prunk, B. Sc.
18. Katja Škrlec, B. Sc.
19. *Maja Štalekar, B. Sc., left 01. 05. 14*
20. Simon Žurga, B. Sc.

### Technical and administrative staff

21. Darja Žunič Kotar

Note:

\*part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Petra Avanzo Caglič, Miha Renko, Dušan Turk, Janko Kos, Jerica Sabotič, "Fungal  $\beta$ -trefoil trypsin inhibitors cnispin and cospin demonstrate the plasticity of the  $\beta$ -trefoil fold", *Biochimica et biophysica acta, Proteins and proteomics*, vol. 1844, issue 10, pp. 1749-1756, 2014.
2. Špela Baebler, Kamil Witek, Marko Petek, Katja Stare, Magda Tušek-Žnidarič, Maruša Pompe Novak, Jenny Renaut, K. Szajko, D. Strzelczyk-Żyta, W. Marczewski, Karolina Morgiewicz, Kristina Gruden, Jacek Hennig, "Salicylic acid is an indispensable component of the Ny-1 resistance-gene-mediated response against Potato virus Y infection in potato", *J. Exp. Bot.*, vol. 65, iss. 4, pp. 1095-1109, 2014.
3. Aleš Berlec, Borut Štrukelj, "A high-throughput biliverdin assay using infrared fluorescence", *J. Vet. Diagn. Invest.*, vol. 26, no. 4, pp. 521-526, 2014.
4. Vesna Brglez, Anja Pucer Janež, Jože Pungerčar, Gérard Lambeau, Toni Petan, "Secreted phospholipases A<sub>2</sub> are differentially expressed and epigenetically silenced in human breast cancer cells", *Biochem. biophys. res. commun.*, vol. 445, no. 1, pp. 230-235, 2014.
5. Boris Brus, Urban Košak, Samo Turk, Anja Pišlar, Nicolas Coquelle, Janko Kos, Jure Stojan, Jacques Philippe Colletier, Stanislav Gobec, "Discovery, biological evaluation, and crystal structure of a novel nanomolar selective butyrylcholinesterase inhibitor", *J. med. chem.*, vol. 57, issue 19, pp. 8167-8179, 2014.
6. Tanja Dreo, Manca Pirc, Živa Ramšak, Jernej Pavšič, Mojca Milavec, Jana Žel, Kristina Gruden, "Optimising droplet digital PCR analysis approaches for detection and quantification of bacteria: a case study of fire blight and potato brown rot", *Anal. bioanal. chem.*, vol. 406, issue 26, pp. 6513-6528, 2014.
7. Anahid Jewett, Yan-gao Man, Nicholas Cacalano, Janko Kos, Han-Ching Tseng, "Natural killer cells as effectors of selection and differentiation of stem cells: role in resolution of inflammation", *J. immunotoxicol.*, vol. 11, no. 4, pp. 297-307, 2014.
8. Marjetka Kidrič, Jerica Sabotič, Branka Stevanović, "Desiccation tolerance of the resurrection plant *Ramonda serbica* is associated with dehydration-dependent changes in levels of proteolytic activities", *J. plant physiol.*, vol. 171, issue 12, pp. 998-1002, 2014.
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# DEPARTMENT OF ENVIRONMENTAL SCIENCES

## O-2

*The activities in the Department of Environmental Sciences are as diverse and varied as the environment itself. They are multidisciplinary, from different natural sciences to social sciences, in particular, chemical, physical, geological and biological, which define our environment, society, and human activities. With our research work we want to clarify the relationship between natural processes and human activities, and the influence of these activities on human health and the environment. The scope of our studies, the educational and technological aspects of research and development are thematically described in the following sections: Environmental analytical chemistry, Biological and geochemical cycles, Environment, nutrition, health, Environmental monitoring, Clean technologies and waste management, Risk and environmental impact assessment.*

### Environmental analytical chemistry

Polybrominated diphenyl ethers (PBDEs) are flame retardants, which, due to their widespread use, are frequently present as pollutants in the environment. In the EU Water Framework Directive (WFD) six PBDE congeners (BDE 28, BDE47, BDE 99, BDE 100, BDE 153 and BDE 154) are listed as priority substances. An analytical procedure for the determination of six PBDE congeners in environmental waters was developed. The limits of quantification (LOQ) for the  $\Sigma$ PBDE, which was found to be  $0.109 \text{ ng L}^{-1}$ , fulfilled the requirements of the WFD.

Within the frame of the metrological EU project WFD, an analytical procedure was optimized for the determination of tributyltin compounds (TBT) in surface waters with the use of gas chromatography (GC) coupled to ICP-MS. For the TBT cation the limit of detection (LOD) was  $0.2 \text{ ng L}^{-1}$ , as required by the Water Framework Directive.

As part of new research activities an investigation of the fate of nanoparticles in the environment was started. For this purpose, an analytical procedure for the quantitative determination and size distribution of  $\text{TiO}_2$  NPs in anatase and rutile was developed, implementing a new approach by using the single particle (SP)-ICP-MS. This procedure also enabled a simultaneous determination of the dissolved titanium concentrations. Different nanosized  $\text{TiO}_2$  NPs, i.e., anatase and rutile, were studied. The procedure developed was applied in the sizing and the determination of the  $\text{TiO}_2$  concentrations in water samples of the Sava River.

In the field of the analysis of organic compounds we devoted most of our research in 2014 to studying the fate of pharmaceutical and personal-care product residues in environmental and wastewater samples, and sediments. The compounds of interest included representative, non-steroidal antiinflammatory drugs, lipid regulators, hormones, tranquilisers, antidepressants, cytostatics, and industrial compounds that produce an endocrine-disrupting effect. To improve the sampling, we improved our own passive sampling method for selected pharmaceuticals and have applied it to surface and ground waters.

Lipid analysis and stable isotopes were introduced to better understand the Neolithic pottery assemblage from the Hočevarica site. The total lipid extracts were subjected to high-temperature gas chromatography (HT-GC), gas chromatography-mass spectrometry (GC-MS) and gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS). The results show that some vessels were used for preparing ruminant meat and vegetables. In some vessels aquatic food was identified. The processing of non-ruminant meat was detected in a few samples. A large number of pottery samples yielded the presence of beeswax lipids.

In order to identify the possible sources of soil  $\text{CO}_2$ , we developed a method for the continuous and fully automated measurements of  $\text{CO}_2$  fluxes within the profile and the simultaneous measurements of the diffusivity of the soil air. Furthermore, the system enables measurements of the isotopic composition of the soil  $\text{CO}_2$  and the  $^{222}\text{Rn}$  activity concentration.

Participation in inter-laboratory comparison studies FIT-PTS was organised by EUROFINs, which include Stable isotope measurements of different foodstuffs.

In the area of chemical metrology the certification of trace elements in candidate Certified Reference Materials for the EU, JRC, Institute for Reference Materials and Measurements (IRMM): (i) Determination of minor chemical elements in TiAlV4 alloy, (ii) Determination of the element



Head:  
**Prof. Milena Horvat**

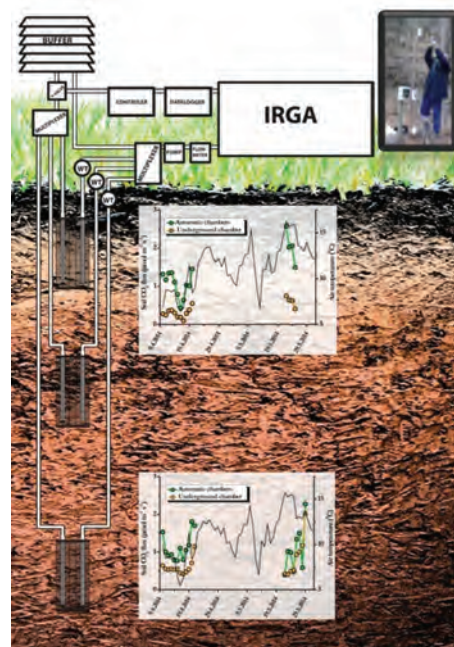


Figure 1: Automatic subterranean chambers for soil  $\text{CO}_2$  concentrations and soil  $\text{CO}_2$  flux measurements. Chambers are placed at different depths within the soil profile, where soil  $\text{CO}_2$  concentrations are measured.  $\text{CO}_2$  fluxes are calculated by the gradient method based on Fick's first law. This apparatus is mounted on soils above the Postojna cave, with aim being to find out if cave air ventilation affects soil  $\text{CO}_2$  fluxes.

mass fraction in pure copper ERM-EB074 A-B-C and (iii) Determination of element mass fraction in copper with added impurities ERM-EB075 A-B-C and BAM/GDMB (Germany), IAEA-MEL (Monaco) and INCT (Poland): Yttrium Stabilized Zirconium Oxide (ERM-ED105), Determination of trace elements and methyl mercury in Oyster in MODAS-2 Bottom Sediment, respectively. 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 also planned in 2015, which will be later entered in the KCDB (*Key Comparisons Data Base*). Furthermore, we participated in inter-laboratory comparison studies organised by IRMM, IAEA, APLAC, TUBITAC UME, NPL and other reference laboratories as well as being involved in their organization.

In the framework of the EMRP project ENV02 dealing with Hg traceability issues in car-exhaust measurements the methods for the determination of Hg and its compounds in exhaust were investigated. It was found that the levels in gasoline and diesel were below the LOD. Moreover, a method for continuous measurements of dissolved gaseous Hg and reactive Hg in natural and industrial waters was developed. A method for the determination of MeHg using hydration as derivatization method at the pg/L level was validated for natural waters.

The scope of accredited methods was described more precisely in the accreditation certificate LP-090 to fulfil the requirements of the Metrology Institute of the Republic of Slovenia (MIRS) for the holders of national measurement standards and of the European Association of National Metrology Institutes (EURAMET). The quality-management system of the Department O2 was re-evaluated and successfully defended at a meeting of the EURAMET Technical Committee – Quality (TC-Q) in Cavtat, Croatia.

### Biological and geochemical cycles

Our research performed in the Gulf of Trieste confirmed that, on an annual scale, the Gulf acts as a sink of CO<sub>2</sub> that is strongly controlled by the seasonal variability of the water temperature, biological processes, wind speed and riverine inputs. The results also indicated that the buffer capacity of the Gulf of Trieste is relatively high, meaning that its waters are not particularly exposed to acidification processes. The combined use of salinity, nutrient concentrations, and nitrate, particulate nitrogen and carbon isotopic compositions revealed that the seawater surface was influenced by mixing with different sources, including seawater, rivers and sewage effluent. Besides mixing, the phytoplankton uptake was the main process controlling the distribution and isotopic composition of NO<sub>3</sub><sup>-</sup> in the marine system. In addition, our results are consistent with the occurrence of nitrification in the water column in autumn and winter.

In collaboration with the National Centre for the Research of Human Evolution (Burgos, Spain), the mechanisms

that transfer the variations in surface atmospheric temperature into caves were studied to evaluate whether they already record the warming trend of recent decades. The study was conducted in Pisani rov, a dead-end isolated gallery of Postojna Cave. A thermal conduction model was implemented that reproduced the low-frequency thermal gradients similar to those measured in the cave atmosphere. The model confirmed that at a depth of 37 m, the bedrock is already recording the local expression of global warming with a delay of 20 to 25 years. In addition, the influence of cave ventilation on the soil CO<sub>2</sub> fluxes was studied at the same location. At the control plot the soil CO<sub>2</sub> fluxes were in a good, positive correlation with the soil temperatures. The soil CO<sub>2</sub> fluxes at the plot above the cave did not show statistically significant correlations with the soil temperatures or the soil moisture, indicating that other factors, possibly cave ventilation, could have an influence.

Within the frame of the EU 7<sup>th</sup> Framework programme GLOBAQUA the first sampling campaign was performed on the Sava River. Together with partners from the Siniša Stanković Institute from Belgrade, water, sediment and biota samples were collected. The preliminary data will serve for the subsequent planning of the sampling strategy and research activities. Moreover, a three-dimensional (3D) model of the Ljubljansko polje aquifer has been constructed using FEFLOW® 6.1. The model will not only present the hydrodynamics of the groundwater, but also the transport of conservative tracers such as δ<sup>18</sup>O, δ<sup>2</sup>H in <sup>3</sup>H. It was found that according to the geological composition of the studied area, a 5-layer model is the most appropriate. The impermeable hard pan of Ljubljansko polje is composed of Permian and Carboniferous rocks, which represent the lower boundary of the model. The surface was generated with a digital elevation model 100 × 100 m, the Sava's alluvial plain with LIDAR 20 × 20 m and the Sava's bathymetry with the cross-sections of the Sava scanned in 2007 and 2010. The model is going to be validated with <sup>3</sup>H/<sup>3</sup>He data, which are available for three locations: Kleče, Hrstje and Jarški Prod.

In the frame of water-cycle investigations we continued our study of the isotopic composition of precipitation at nine stations in Slovenia in cooperation with IAEA and Slovenian Environmental Agency (ARSO). These stations have been included into the Global Network of Isotopes in Precipitation (GNIP) since 2013. We collaborated with researchers from the University of Ljubljana and

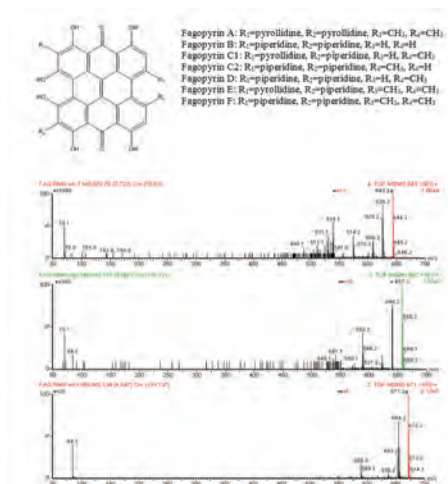


Figure 2: The figure shows the results of spectroscopic determination of possible structures of phototoxic compounds fagopyrins and its derivatives that have been isolated from buckwheat herb. From the MS-MS spectra of ions at molecular mass: 643, 657 and 671

Da the derivatives Fagopyrin A, C and E have been recognized, respectively. These are poorly investigated compounds sensitive to daylight, which expressed after ingestion of large amounts of buckwheat as skin irritations, so-called fagopyrim.

the Institute of Geography at the Russian Academy of Sciences in the evaluation of a 30-years-long isotope record for Ljubljana and estimated the relation between the isotopic composition of the precipitation and the atmospheric circulation patterns. The spatial variability of the stable-isotope composition of the precipitation and the snow, and their influence on the surface runoff and groundwater in north-western Slovenia was investigated. The obtained data on the isotopic composition of the precipitation, surface and groundwater, the snow and the snowmelt will be used in a further improvement of the water balance model of the Julian Alps. Also within an IAEA project, the testing of passive capillary samples to collect snowmelt water for isotope analyses was performed at 11 sites in ten partner countries in different climates, and recommendations for constructing and installing the PCS for the snowmelt sampling for isotopic analysis were prepared.

In the frame of a USA-Slovenia bilateral cooperation we studied stream carbon controls in seasonally snow-covered mountain catchments: the impact of the inter-annual variability of water fluxes, the catchment aspect and the seasonal processes. We elucidated the impact of: (i) changes in water flux (by comparing years of variable wetness), (ii) catchment aspect [north-facing (NF) vs. south-facing (SF)] and (iii) season (snowmelt vs. summer) on the dissolved organic carbon, chromophoric dissolved organic matter and dissolved inorganic carbon in forested catchments within the Valles Caldera National Preserve, New Mexico.

Based on the stable isotope compositions of carbon and oxygen for shells and soft tissues, invasive serpulids (*Ficopomatus enigmaticus*) in the Krka estuary (Croatia) were proven to be excellent environmental indicators of salinity and sources of particulate and dissolved nutrients, and can be therefore be used as proxies for water circulation in a permanently stratified microtidal estuary.

In collaboration with the Ruder Bošković Institute (Zagreb) and the Institute for Oceanography and Fisheries (Split, Croatia), geochemical and isotopic analyses, as well as biological parameters (condition index, gonadosomatic index) were used to study the nutrient and contaminant transfer and nutrition sources of filtering organisms along the Adriatic Coast for the case of different cultured and wild populations of mussels. A multidisciplinary approach was used to estimate the pollution level of the marine environment in the Gulf of Trieste. The presence of sewage sludge was not confirmed, while elevated concentrations of Cu, Zn, and Pb in mussels were only found in the Bay of Koper. The feeding ecology of the commercially important co-occurring bivalves in the Mali Ston Bay (Central Adriatic) were investigated using isotope ratios and lipid content in different tissue types. It was found that isotopic niche overlap (up to 60 %) among the cultured species (*Mytilus galloprovincialis* and *Ostrea edulis*) was the highest during the spring–summer period, while for wild species (*Modiolus barbatus* and *Arca noae*), the overlap was the highest in the autumn–winter period, which is important for the sustainable management of cohabiting wild and cultured species. In collaboration with the University of Haifa (Israel), the competition for resources between common bottlenose dolphins (CBD) and bottom trawlers was investigated. The stable isotope ratios of C and N in the muscle tissues of different organisms showed that the sharing of resources is much smaller than expected; therefore, CBDs have a minor overall effect on the bottom fish trawlers, mainly in the Sparidae catch.

In cooperation with the Velenje Coal Mine, the sources and distribution of coalbed gases were determined in relation to the longwall method of excavation in the mining areas of Preloge and Pesje. The geochemical and isotopic compositions of the surface waters and the groundwater in the Velenje Basin were investigated seasonally to determine the relationship between the major aquifers and surface waters, the water-rock interactions, the relative ages of the groundwater, and the biogeochemical processes.

The partitioning of natural radionuclides in sediments and streams affected by the waste piles of the former uranium mine and mill located at Žirovski vrh, Slovenia, was performed by applying a sequential extraction procedure. The results definitely showed that the total activity concentrations at the sites downstream of the influence of the waste piles were higher than at the sites upstream of the piles. This difference was geographically very limited to a distance of about 5 km downstream. The fractionation of radionuclides upstream and downstream of the area of influence of the waste piles did not appear to be significantly altered.

New data on the concentrations of the main gamma-emitting radionuclides, minor and trace elements, and isotopes of uranium and thorium in soils and sediments of the Shu valley, Kazakhstan, were determined. The results obtained showed the aquatic migration pathway of most of the trace elements and radionuclides and predicted the water pollution down-stream of the river Shu. Pollution by particular trace elements was revealed, and areas with accumulation and leaching processes were estimated by the disequilibrium isotopic method for uranium.

An integral radiological survey was carried out in the area of former uranium and mill located at Žirovski vrh, Slovenia: the mobility and bioavailability of the uranium-radium decay chain radionuclides were assessed. The mobility of the radionuclides in the soil was assessed by applying a sequential extraction procedure. The most mobile appeared to be the uranium radionuclides, followed by  $^{226}\text{Ra}$  and  $^{230}\text{Th}$ , being the least-mobile radionuclide. The wetland plants grown in soils contaminated with seepage waters from the tailings contained higher levels of the above-mentioned radionuclides compared to plants from a control site.



We investigated Se concentrations and its chemical species in macrophyte *Veronica anagallis-aquatica* and river sediments in three Slovenian streams that flow through the agricultural area. *Veronica anagallis-aquatica* was chosen because it is an amphibious plant, widely distributed in Slovenia.

In the framework of the EU project GMOS, measurements of mercury speciation in the marine environment continued, accompanied with a Hg determination in air and precipitation. Moreover, in collaboration with the institute of oceanography and fisheries in Split, the seasonal variation of mercury speciation was studied in the central Adriatic Sea. The main purpose is to study the effect of marine biology on the mercury cycle.

#### Environment, nutrition, health

In collaboration with the Chemical Office of the Republic of Slovenia, University Medical Centre Ljubljana, regional institutes of Public Health, regional hospitals and health we continued national human biomonitoring. We analysed toxic chemicals, including toxic metals (cadmium, lead, mercury) and persistent organic pollutant, including dioxins, pesticides, PCBs, polybrominated flame retardant in human blood, urine and maternal milk. The results will be used for an assessment of the burden of the Slovenian population with these environmental pollutants. The regular monitoring programme comprised measurements for updating the database on the isotopic composition of Slovenian wines in accordance with EU regulations, and the isotopic composition of the precipitation in Slovenia.

In two "exposome" projects funded by the EU, i.e., the LIFE12ENV/-CROME-LIFE; Cross-Mediterranean Environment and Health Network, 2013–2016 and HEALS, Health and Environment-wide Associations based on Large population Surveys, 2013 – 2017, a methodological framework was completed.

Knowing the pharmacokinetics of chemotherapeutics in serum contributes to the optimization of cancer treatments. By applying conjoint liquid chromatography (CLC), which enables the simultaneous two-dimensional separation of ionic forms of metal-based chemotherapeutics from the portions bound to serum proteins and using UV and inductively coupled plasma mass spectrometry (ICP-MS) for detection of separated metal species, the kinetics of the binding of new ruthenium compounds to human-serum proteins was investigated. In collaboration with co-workers from the Oncology Institute and the Faculty of Chemistry and Chemical Technology, modulation of the activity of the known cytotoxic ruthenium(III) compound (KP418) with hampered transmembrane transport in electrochemotherapy was studied *in vitro* and *in vivo*.

Fish, shells and molluscs are the main pathways of human exposure to organotin compounds (OTC). Since there is a lack of data available on the occurrence of OTC in these foodstuffs, which are available on the Slovenian market, the presence of OTC was checked in different marine and freshwater fish farms from Slovenia, Turkey, Bosnia and Herzegovina and Italy. In 36 % of samples analysed from the marine organisms the presence of TBT was confirmed, while in 13.6 % of samples, elevated concentrations of dibutyltin were found. However, the concentrations of OTC determined were low and did not pose any risk to human health.

Selenoproteins and metallothioneins (MTs) mRNA expression was studied in a small group of Idrija residents occupationally and/or environmentally exposed to inorganic mercury, mostly in vapour form. The gene expression of six MT (sub)isoforms, i.e., MT2a, MT1 (a,e,f,x) and MT3, together with four selenoproteins, was followed by qPCR. The suppressed gene expression of MT1f and MT1x should be studied on a wider group of Idrija residents to confirm the observed phenomenon of suppression.

We exploited the results of a 10-years-long study on arsenic trioxide (ATO) treated patients. Arsenic metabolites and selenium levels in the serum and urine of acute promyelocytes leukemia (APL) and multiple myeloma (MM) patients treated by ATO have shown that MM patients were undertreated regarding the concentrations of the active compound (arsenite), but also at greater risk for treatment side effects due to the more-or-less severe selenium deficiency present before treatment or acquired during treatment.

Regarding arsenic speciation the difference between benthic (*Pteromylaeus bovinus*, *Myliobatis aquila*) and pelagic rays (*Pteroplatytrygon violacea*) from the northern Adriatic Sea (Gulf of Trieste) in relation to their size (age) was investigated. High arsenic concentrations were found in both groups, with a tendency for a more efficient arsenic accumulation in the benthic species, particularly in the muscle (32.4 to 362  $\mu\text{g g}^{-1}$  of total arsenic). The good correlations between the total arsenic/arsenobetaine and the size reflect the important accumulation of arsenobetaine with age. Arsenobetaine is an analogue of glycine betaine, a known osmoregulator in marine animals and both are very abundant in mussels (*Mytilus galloprovincialis*), representing an important source of food for benthic ray species. We have also studied the contents of arsenic and its compounds in cooked rice compared to raw rice, because of the indigenous cooking in the households of rural Bengal. The results indicate that inorganic arsenic is the predominating species in both raw and cooked rice. The cooking of rice with an excess of clean water ( $<10 \mu\text{g As L}^{-1}$ ) significantly decreases the total and inorganic arsenic content in cooked rice compared with raw rice, while untreated, arsenic-contaminated water increases the arsenic content in cooked rice. The washing of rice grains with clean water removes the negligible amount of arsenic from the grains. The assessment of the arsenic exposure risk indicates that despite a significant decrease of the arsenic contents in cooked rice, still for

more than 10% of the surveyed participants have a daily intake of inorganic As through the consumption of cooked rice (DI-As-CR) that exceeds the previous provisional tolerable daily intake (PTDI) value recommended by World Health Organization (WHO).

Iodine is an essential element for humans and other mammals. The newly developed ICP MS technique was used for a determination of the iodine concentrations in pea sprouts, buckwheat sprouts and pumpkin sprouts that were germinated from seeds soaked in the iodide or iodate solution. The plants were chosen from different groups – pulses, pseudo-cereals and oilseed plants. In addition, the adult plants as well as sprouts are used in the nutrition. We found that the iodine uptake for all plants is very effective, irrespective of the added form of iodine. No significant differences in the amount of iodine in plants were found between the iodide- and iodate-treated plants for pea sprouts and pumpkin sprouts. In buckwheat sprouts a higher amount of iodine was found in plants treated with iodate in comparison with those treated with iodide.

Stable isotope and elemental parameters were used to determine the geographical origin of Slovenian fresh apple juice. The regional assessment of apple-juice samples was the most successful when  $\delta^{15}\text{N}$  and  $\delta^{13}\text{C}$  in pulp;  $\delta^2\text{H}$  and  $\delta^{18}\text{O}$  of fruit juices water using IRMS (Isotope Ratio Mass Spectrometry); (D/H)<sub>I</sub> and (D/H)<sub>II</sub> in ethanol by SNIF-NMR (Site-specific Natural Isotopic Fractionation Nuclear Magnetic Resonance) were combined with S, Cl, Fe, Cu, Zn and Sr. The overall prediction ability was 83.9%.

The first database for authentic Slovenian cow, sheep and goat milk and cheese was established. The database includes the isotope parameters ( $\delta^{18}\text{O}$ ,  $\delta^2\text{H}$  values) in milk, isotopic composition of carbon and nitrogen in casein, the content of fatty acids and elemental composition. The results of the research and statistical analyses indicate that the use of stable isotopes in a combination with the elemental composition is the most appropriate approach for the verification of the declared geographical origin. Furthermore, they are also useful in separating the sheep and goat milk and cheese from cows. Due to the fact that with these parameters the area of production of sheep's milk or cheese could be identified, a proper database can be used to protect the geographical origin of Bovški and Kraški cheese. The parallel investigation of goat and sheep chesses by real-time PCR and fatty acid composition indicate that both methods are comparable for detecting adulteration and when the addition of cow's milk to sheep or goat milk is greater than 5%. In addition, the adulteration of raw cow milk with less than 5% vegetable palm tallow was easily detected, due to the difference in the fatty acids composition. Furthermore, it was found that on the Slovenian market the largest mislabellings are present for goat and sheep chesses. It was found that 20% of them do not correspond to the declaration.

In collaboration with the University of Venice a study of the influence of climate change on the quality of Italian wine products was performed. In this study the complementary methods of IRMS and SNIF-NMR were used, since the fractionation of stable isotopes of C, O and H are related to temperature changes and thus to climate change.

The geographical origin of underground and mineral waters as well as agricultural crops and products, can be followed by the determination of the isotopic ratio of  $^{87}\text{Sr}/^{86}\text{Sr}$ . In this new field of research, the analytical procedure for the isolation of strontium from the matrix was optimized by the use of extraction chromatography on strontium selective resin. The isotopic ratio  $^{87}\text{Sr}/^{86}\text{Sr}$  was determined on quadrupole ICP-MS. The first results revealed that in waters with a different isotopic ratio  $^{87}\text{Sr}/^{86}\text{Sr}$  the water origin could be predicted.

Based on results of previous investigations of the isotopic composition of bottled waters we analysed, together with researchers from the University of Ljubljana and the Geological Survey of Slovenia, the applicability of deuterium excess in bottled water life cycle was investigated. It was shown that deuterium excess can be used as an additional tool in the authentication of bottled waters.

The activity concentrations of uranium-radium decay chain radionuclides in tap waters, originating from various geological regions of Croatia were determined. Based on those measurements, the average total annual internal doses for infants, children and adults, as well as contribution of each particular radionuclide to total dose, were assessed. The highest doses were calculated for infants, which makes them the most critical group of the population. However, all the values for each population group were well below the recommended reference dose level from the consumption of the drinking water according to the EU. The lowest contribution to the total dose was found for  $^{226}\text{Ra}$  and the highest for  $^{228}\text{Ra}$ .

Radon ( $^{222}\text{Rn}$ ) has been investigated in the air of dwellings and in a karst cave. Because carbonate bedrocks (with high radon potential) cover more than half of Slovenia, they are crucial for the increased radon risk in buildings. A year-long study was performed in an older house in the Slovenian karst area, with a mean radon level of  $\text{kBq m}^{-3}$ . The concentration of radon and meteorological parameters were followed continuously, at hourly intervals, in the ground- and first-floor living rooms. The influence of the meteorological conditions on the radon entry into the

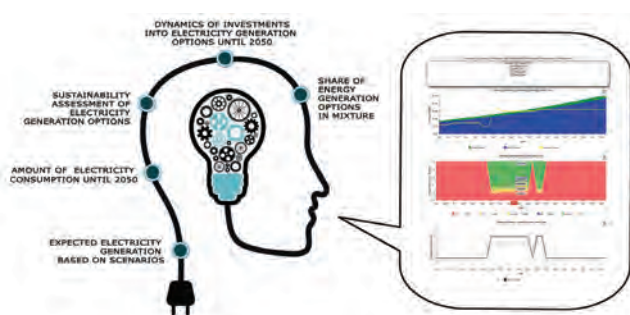


Figure 3: Illustration of the evaluation of electricity-generation scenarios

building and its spreading to upper floors has been sought. However, our main interest was the radon dosimetry. It was found that the dose estimation, based on the annual or semi-annual radon concentration, instead of daily or hourly radon concentrations, is justified. As part of a long-term study, radon was also continuously monitored in the poorly ventilated Gaily Coloured Corridor of the Postojna Cave.

Research on nano-aerosols has been continued. In collaboration with other research institutions in Slovenia (University of Nova Gorica, Aerosol Company, and the Department of Condensed Matter Physics at the JSI) extensive measurements of nanoparticles and black carbon were carried out in outdoor air. Complex research on nano-aerosols in indoor air with increased concentrations of radioactive aerosols (radon and thoron decay products) was focused on the impact of radioactive aerosols on the creation and distribution of small negative and positive air ions (<1 nm) and on the size distribution and number concentration of background nano-aerosol particles (5–350 nm). This research was performed in Niška Banja, Serbia, the place of increased indoor radon and thoron levels.

For the first time, radon was systematically surveyed in more than 100 tap-water supply plants, selected on the basis of hydrology and density population in Slovenia. In contrast to indoor radon, the results ranked us among the countries with a low radon risk in drinking water.

Within the EU 7FP CITI-SENSE project (Development of sensor-based Citizens' Observatory Community for improving quality of life in cities) as part of the empowerment initiatives sensors and information infrastructure for continuous monitoring of air quality was tested at selected outdoor locations in Ljubljana, as well as indoor air in two schools (Gimnazija Vič and Sp. Šiška elementary school) and mobile AQ units based on the participatory principle during the movement of people.

### Environmental technologies

In collaboration with the Slovenian Building Institute the efficiency of the removal of Zn<sup>2+</sup>, Zn-EDTA and Zn-citrate from aqueous solutions by the use of nanoscale zero-valent iron was investigated. The study importantly contributes towards an understanding of the interactions between positively charged ionic zinc species and iron nanoparticles and also to understand the behaviour of negatively charged zinc complexes within the presence of iron nanoparticles. From the results of the investigation it was possible to optimize the conditions for the effective removal of zinc species from contaminated waters.

Within the frame of the EU project RusaLCA in collaboration with Slovenian Building Institute, we continued with the optimization of the remediation of wastewater from small biological treatment plants. The procedure is based

on the use of nano-zerovalent iron in combination with ion-exchange column and adsorbing agents. It enables the efficient remediation of wastewater, which fulfils the requirements for drinking water. Together with co-workers from the Slovenian Building Institute different ways of remediation of highly contaminated soil from Celje basin were investigated.

In the field of the chromium speciation inhibition of the nitrification process in activated sludge by trivalent and hexavalent chromium and the partitioning of hexavalent chromium between the sludge compartments was investigated. A critical overview of Cr speciation analysis based on high-performance liquid chromatography and spectrometric techniques was also published.

A procedure was developed for the micro-scale synthesis of <sup>117</sup>Sn-enriched tributyltin chloride from <sup>117</sup>Sn-enriched metallic tin. The isotopically enriched tin tracers: namely <sup>117</sup>Sn-enriched tributyltin (TBT), <sup>119</sup>Sn-enriched dibutyltin (DBT), <sup>117</sup>Sn-enriched SnCl<sub>2</sub>, <sup>117</sup>Sn-enriched SnCl<sub>4</sub> and a <sup>119</sup>Sn-enriched butyltin mix containing TBT, DBT and monobutyltin (MBT), were then used to follow the transformation of organotin compounds (OTCs) in landfill leachate. The OTCs were quantified by the GC-ID-ICP-MS. To discriminate the biotic and abiotic transformations of OTCs and inorganic tin species, the sterilization of leachate was also performed and the data were compared to

non-sterilized samples. During the course of the experiment the microbial degradation of TBT was clearly manifested in Sn-enriched spiked leachate samples, while the abiotic pathway of the degradation was observed for DBT. The biomethylation process was also observed in the leachate spiked with Sn-enriched Sn<sup>2+</sup> or Sn<sup>4+</sup>. The results of the present investigation importantly contribute to a better understanding of the processes that OTCs undergo in leachates, and provide useful information to managers of landfills when taking measures necessary to prevent the release of toxic methyltin species into the nearby environment.

In the area of cytostatic research within the FP7 project CytoThreat, we developed a series of analytical procedures for determining cytostatics (5-fluorouracil, capecitabine, cyclophosphamide, ifosfamide, methotrexate, imatinib,



*Figure 4: Within the EU 7th Framework project GLOBAQUA the first sampling campaign was performed on the Sava River. Together with partners from the Siniša Stanković Institute from Belgrade, water, sediment and biota samples were collected.*

vincristin and etoposide) and their commercially available metabolites in waste and environmental water samples. We also investigated their presence in hospital and municipal wastewaters and in receiving surface waters. Through our work we show the presence of detectable quantities of these compounds in wastewaters from hospitals, where cancer therapies are being conducted and in wastewater-treatment plant (WWTP) influents. None of the studied cytostatics were detected in WWTP effluent and their receiving waters. We also studied the bio- (suspended and attached biomass) and photodegradation of selected cytostatics and their metabolites and endocrine-disrupting compounds where our group was the first to identify several novel transformation products formed during these processes. In addition we studied cavitation, a novel AOP, as a viable option to remove organic micro-pollutants like pharmaceuticals (anti-inflammatory drugs, tranquilisers, hormones, cytostatics) and endocrine disrupter compounds (BPA, parabens and triclosan) from wastewaters. In addition, we have started with the development of molecular imprinted polymers and their application within environmental bioanalytics as well as studying the cycling of bisphenol A (BPA) and its alternatives from food to wastewaters and the environment.

In collaboration with the Department of Inorganic Chemistry and Technology we continued our research on cost-effective methodologies for the removal of mercury in flue gases by the oxidation method in flue-gas desulfurization plants. Mathematical models were introduced and used for the simulation of aqueous Hg chemistry. Mercury behaviour in solid samples at higher temperatures was also studied as part of the initial experiments for the removal of Hg from gases at higher temperatures.

### **Risk and environmental impact assessment**

The most complex work in 2014 was the finalization of the study "Sustainability appraisal of energy policy development of Slovenia by 2030" followed by an illustrative brochure aimed at informing the general public about the results of the study. In the framework of consultancy work technical support in the permitting processes for Slovenian Seveso lower tier establishment has been provided for the Ministry of the Environment and Spatial Planning - Environmental Agency. Additionally, technical guidelines for industrial accidents risk prevention in the phase of spatial plan preparation for the business zone Litostraj in Ljubljana have been developed. In terms of international cooperation the activities were related to the IAEA Coordinated Research Project "Techno-economic Evaluation of Options for Adapting Nuclear and Other Energy Infrastructure to Long-term Climate Change and Extreme Weather".

### **Environmental Monitoring**

The regular monitoring programme comprised measurements for updating the database on the isotopic composition of Slovenian wines in accordance with EU regulations.

In collaboration with the Environmental Agency of the Republic of Slovenia monitoring of organotin compounds in surface and sea water was continued in 2014. Gaseous mercury in the air and in precipitation was also implemented at the EMEP background station at Iskrba.

The monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski vrh was performed. We participated in Off-Site Monitoring of the Krško Nuclear power plant by determining the strontium and tritium in environmental samples. Also, we determined the tritium and C-14 in gas effluents from the nuclear power plant. Using methods are accredited by the Slovenian accreditation body (SA LP-090).

### **Infrastructure activities**

Infrastructural Center for Mass Spectrometry (CMS) which operates within the Department of Environmental Sciences and with the mass spectrometric measurements participated in many research programs: the circulation of substances in the environment, chemistry for sustainable development, functional foods and dietary supplements, synthesis and transformation of organic compounds, and bioinorganic and bioorganic chemistry, design, synthesis and evaluation of active planning and preclinical development of new active pharmaceutical compounds, pharmaceutical biotechnology, chemistry and structure of biologically active compounds, functional genomics and biotechnology for health, toxins and biomembrane, proteolysis and its regulation, molecular biotechnology, promoted by JSI, National Institute of Chemistry, National Institute of Biology, University of Ljubljana, Maribor and Nova Gorica, Centers of excellences: En-fist, CIPKeBiP, and Namaste. With a high-resolution tandem mass spectrometry QToF Premier and LC-MS analytical system were also identified and structurally characterized a number of organic compounds, organic-metal complexes, and biopolymers in the field of speciation and interactions of chemical pollutants in aqueous solutions, toxic metals and organometallic compounds in the terrestrial environment, metabolites active substances in advanced water treatment with ultrasound and cavitation, peptides, proteins and other biomarkers in metabolomics, metagenomics and changes in lipid membrane diseases.

The wide application of mass spectrometry has enabled support for the CMS in the research and development of new synthesized organic compounds, active ingredients, proteins and other biomolecules, materials in ceramics, electronics, energy, quality control of food, monitoring pollutants in the environment and assessing their impact on human health, etc.



The Department of Environmental Sciences also operates a mobile chemical laboratory ELMU (ecological laboratory with a mobile unit), which is organized in a system of Slovenian Civil Protection as a unit for intervention in ecological accidents with hazardous substances and materials, determining the parameters of the field, to assess the impact of pollution on the environment and human health and consultation to neutralisation of the effects of pollution. The chemical mobile unit had six interventions in 2014, mainly due to chemical accidents and the environmental pollution of toxic compounds. Last year was historic for the ELMU because we received new vehicle, a Fiat Ducato, which was in the autumn upgraded to a modern mobile laboratory. The upgrade of the vehicle included the installation of ceiling, floor and wall insulation, electrical and additional lighting installation, air-conditioning of the laboratory place of vehicle and installation of laboratory equipment: desk, built-in cabinets and shelves for storage and installation of instruments, equipment, technical units, and refrigerator for sample storage in mobile chemical laboratory.

### Some outstanding achievements

1. Study of the conversions of organotin compounds in samples of leachate from landfills has significantly contributed to our understanding of the transformation processes in the OTC leachate, which help to design appropriate measures to prevent the release of toxic compounds methyl-tin compounds into the environment. The results of these studies were published in the prestigious journal *Water Research*.
2. In April 2014, a Group for modelling, risk assessment and evaluation of interventions in the environment completed the task of "Sustainability appraisal of energy policy development of Slovenia by 2030" with a focus on nuclear technology (OVJE).
3. In May 2014, an international workshop entitled "Internal Exposome Markers" was organized, which was attended by 50 domestic and international experts. The workshop was a major step in the design of interdisciplinary research in the field of environment and health HEALS.
4. An EU project ERAChair Iso-food on food quality, safety and traceability using isotopic techniques was approved. The project is intended to strengthen the role of the research institute in the field of nutrition as well as the transfer of knowledge within the framework of international doctoral and postdoctoral training in cooperation with the Jožef Stefan International Postgraduate School.
5. In a series of Handbook of Environmental Chemistry published by Springer, a book *The Sava River* was published, edited by Radmila Milačič and Janez Ščančar from the Department of Environmental Sciences and Momir Paunovic from the Institute for Biological Research Sinisa Stankovic from Belgrade. The book comprises a comprehensive review of the impact of hydropower stations, river transport, intensive agricultural activities, industry, population in concentrated areas and the occurrence of floods and droughts on the environment and biota in the Sava River Basin.
6. During Green Week on 4 June 2014 in Brussels award for the best EU Life + project in 2014 was awarded for the theme of environment, information and communication "Green Week 2014 04 June 2014 - Best LIFE Environment & Information and Communication Projects Award". It was awarded to the DEMOCOPHES project, which was a pilot implementation of a harmonized European human biomonitoring, in which the department was fully involved.
7. Prof. Dr. Milena Horvat was given a Zois award for outstanding achievements in mercury research. Awards for outstanding achievements in the field of environmental research were given to Prof. Dr. Nives Ogrinc and dr. Marko Štok in the field of energy.

### Some outstanding publications in the past year

1. Amos, H. M., Jacob, D. J., Kocman, D., Horowitz, H. M., Zhang, Y., Dutkiewicz, S., Horvat, M., Corbitt, E. S., Krabbenhoft, D. P., Sunderland, E. M.: Global biogeochemical implications of mercury discharges from rivers and sediment burial. *Environmental science & technology*, 2014, 48 (16), 9514-9522.
2. Peeters, K., Zuliani, T., Ščančar, J., Milačič, R.: The use of isotopically enriched tin tracers to follow the transformation of organotin compounds in landfill leachate. *Water Research*, 2014, 53, 297-309
3. Kotnik, K., Kosjek, T., Krajnc, U., Heath, E.: Trace analysis of benzophenone-derived compounds in surface waters and sediments using solid-phase extraction and microwave-assisted extraction followed by gas chromatography-mass spectrometry. *Analytical and bioanalytical chemistry* 2014, vol. 406, 3179-3190, doi: 10.1007/s00216-014-7749-0
4. Jin, L., Ogrinc, N., Yesavage, T., Hasenmueller, E. A., Ma, L., Sullivan, P. L., Kaye, J. P., Duffy, C., Brantley, S. L.: The CO<sub>2</sub> consumption potential during gray shale weathering: Insights from the evolution of carbon isotopes in the Susquehanna Shale Hills critical zone observatory. *Geochimica et cosmochimica acta*, 2014, 142, 260-280, doi: 10.1016/j.gca.2014.07.006

## Awards and appointments

1. Milena Horvat: The Zois Award for superb achievements in the area of scientific, research, and developmental activities in the field of mercury, Ministry of Education, Science and Sport
2. Milena Horvat: Green Week 2014, EU Life+, EU project Democophes; ("Green Week 2014, Best LIFE Environment & Information and Communication projects Award"), Brussels, Belgium, 4 June 2014
3. Marinka Gams Petrišič, Gregor Muri, Nives Ogrinc: Excellence in Science 2013: Source identification and sedimentary record of polycyclic aromatic hydrocarbons in Lake Bled (NW Slovenia) using stable carbon isotopes, ARRS
4. Marko Štrok, Borut Smodiš: Excellence in Science 2013: Soil-to-plant transfer factors for natural radionuclides in grass in the vicinity of a former uranium mine, ARRS

## Organization of conferences, congresses and meetings

1. Milena Horvat: Workshop on Internal Exposome Markers in HEALS, Ljubljana, Slovenia, 26–27 May 2014
2. Ljudmila Benedik: Training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC Enlargement & Integration policy, Ljubljana, Slovenia, 10–21 November 2014
3. Nives Ogrinc: Workshop: The use of specific methods for determination and prevention of adulteration of milk and dairy products, Ljubljana, Slovenia, 12 June 2014

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## INTERNATIONAL PROJECTS

1. Small Services in the Years from 2007 to 2014  
Prof. Milena Horvat  
Foreign buyers
2. Determination of the Isotopic Composition of Carbon in Sugar Samples  
Prof. Nives Ogrinc  
Foreign buyers
3. Provision of Testing Services for Filter Media used in IMS Radionuclide Stations  
Prof. Ljudmila Benedik  
The Preparatory Commission for the Comprehensive Nuclear-Test-Ban Treaty Organization
4. 7FP - ArcRisk; Arctic Health Risks: Impacts on Health in the Arctic and Europe Owing to Climate-induced Changes in Contaminant Cycling  
Prof. Milena Horvat  
European Commission
5. 7FP - GMOS; Global Mercury Observation System  
Prof. Milena Horvat  
European Commission
6. 7FP - CYTOTREAT; Fate and Effects of Cytostatic Pharmaceuticals in the Environment and the Identification of Biomarkers for and Improved Risk Assessment on Environmental Exposure  
Prof. Ester Heath  
European Commission
7. 7FP - CITI-SENSE; Development of Sensor-based Citizens' Observatory Community for Improving Quality of Life in Cities  
Prof. Milena Horvat  
European Commission
8. 7FP - HEALS; Health and Environment-wide Associations Based on Large Population Surveys  
Prof. Milena Horvat  
European Commission
9. 7FP - GLOBAQUA; Managing the Effects of Multiple Stressors on Aquatic Ecosystems Under Water Scarcity  
Prof. Radmila Milačič  
European Commission
10. 7FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability  
Prof. Milena Horvat  
European Commission
11. 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  
Prof. Milena Horvat  
IAEA - International Atomic Energy Agency
12. Use of Environmental Isotopes in Investigations of Influence of Snow Melt on Stream Runoff in the Area of Julian Alps, NW Slovenia  
Dr. Polona Vreča  
IAEA - International Atomic Energy Agency
13. Assessment of Human Milk Intake in Infants Living in Gold Mining Areas in South West Nigeria, using Stable Isotope Techniques  
Dr. Darja Mazej  
IAEA - International Atomic Energy Agency
14. PartEmission; EMRP - Emerging Requirements for Measuring Pollutants from Automotive Exhaust Emissions  
Prof. Milena Horvat  
Euramet e.V.
15. Training in Radiochemistry and Radioactivity Measurements for Practitioners from Countries Eligible under the JRC Enlargement & Integration Policy  
Prof. Ljudmila Benedik  
Institute for Reference Materials and Measurements
16. EMRP; Traceable Measurements for Monitoring Critical Pollutants under the European Water Framework Directive (WFD-2000/60/EC)  
Prof. Radmila Milačič  
Euramet e.V.
17. Techno-economic Evaluation of Options for Adapting Nuclear and Other Energy Infrastructure to Long-term Climate Change and Extreme Weather  
Asst. Prof. Branko Kostić  
IAEA - International Atomic Energy Agency
18. Training Fee for Ms Christiane Odumah Anderson, (Ghana), 1 October-24 December 2012, 8 September-7 December 2013, 26 April-26 July 2014  
Prof. Milena Horvat  
ICTP - Centro Internazionale di Fisica Teorica
19. LIFE12 ENV/ - CROME-LIFE; Cross-Mediterranean Environment and Health Network  
Prof. Milena Horvat  
European Commission
20. LIFE RusaLCA-Nanoremediation of Water from Small Waste Water Treatment Plants and Reuse of Water and Solid Remains for Local Needs  
Prof. Janez Ščančar  
European Commission
21. The Use of Stable Isotopes and Elemental Composition for Determination of Authenticity and Geographical Origin of Milk and Dairy Products; Accessible Technologies for the Verification of Origin of Dairy Products as an Example Control System  
Prof. Nives Ogrinc  
IAEA - International Atomic Energy Agency
22. Determination of Minor Elements in TiAl6V4 Alloy  
Dr. Radojko Jačimović  
Institute for Reference Materials and Measurements
23. IAEA Fellowship for Mr Ilya Samoilov, KAZ/12009, 13 January-12 February 2014  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency
24. IAEA Fellowship for Mr Osama Mhmoed Hamed, SUD/12018, 27 January-26 May 2014  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency
25. Review and Interpret HBM Surveys and Data in Europe  
Prof. Milena Horvat  
World Health Organization
26. Characterisation Study of ERM-EB074 and ERM-EB075  
Dr. Radojko Jačimović  
Institute for Reference Materials and Measurements

27. MeTra; EMRP - Traceability for Mercury Measurements  
Prof. Milena Horvat  
Euramet e.V.
28. Mercury Processes in Aquatic Systems; Mercury Methylation and Reduction in Natural Aquatic Environments: Laboratory Studies using High Specific Activity 197Hg Radiotracer  
Prof. Milena Horvat  
Slovenian Research Agency
29. Where is Radon (Gaseous Soil Component) Coming From?  
Prof. Janja Vaupotič  
Slovenian Research Agency
30. The Impact of Colloidal Particles on the Fate of Trace Elements in Environmental Compartments  
Prof. Radmila Milačič  
Slovenian Research Agency
31. Evaluating the Vulnerability of Groundwater Resources using Groundwater Tracers  
Prof. Nives Ogrinc  
Slovenian Research Agency
32. Lake Ecosystems: Vulnerability to Pollution and Sustainable Development  
Prof. Nives Ogrinc  
Slovenian Research Agency
33. Multicontaminant Removal in Wet Flue Gas Desulphurisation (FGD)  
Prof. Milena Horvat  
Slovenian Research Agency
34. The Role of Microbial Community Structure on Mercury Speciation in the Open Adriatic Sea  
Prof. Milena Horvat  
Slovenian Research Agency
35. Stabilisation and Incorporation of Waste Materials into Composites based on Cement and Fly Ash  
Prof. Janez Ščančar  
Slovenian Research Agency
36. Probabilistic Risk Assessment for Mercury Associated with Food Consumption  
Prof. Milena Horvat  
Slovenian Research Agency
37. Determination of Alpha Emitters in Various Samples with Emphasis on Source Preparation Procedures  
Prof. Ljudmila Benedik  
Slovenian Research Agency
38. Occurrence and Fate of Mercury in the Marine Environment  
Prof. Milena Horvat  
Slovenian Research Agency
39. Environmental Isotopes in Snow Hydrology  
Dr. Polona Vreča  
Slovenian Research Agency
40. ICMGP, International Conference on Mercury as a Global Pollutant  
Prof. Milena Horvat  
Slovenian Research Agency
41. IASWS - International Association for Sediment Water Science  
Prof. Nives Ogrinc  
Slovenian Research Agency
- Environment  
Prof. Ester Heath
7. The Effect of Iodine and Selenium on Growth and Quality of Crops  
Prof. Vekoslava Stibilj
8. Archaeologies of Hunter-gatherers, Farmers and Metallurgists: Cultures, Populations, Palaeoeconomies and Climate  
Prof. Nives Ogrinc
9. Advanced Water Treatment with Ultrasound and Cavitation  
Prof. Ester Heath
10. Groundwater Age Determination in Deep Aquifers of Slovenia  
Prof. Sonja Lojen
11. Sediments in Aquatic Environments: Their Geochemical and Mineralogical Characterization, Remediation, and Use as Secondary Raw Materials  
Prof. Radmila Milačič
12. Optimization and Validation of New Indicator Systems in Complex Environmental Matrices  
Prof. Milena Horvat
13. Evaluating Geological Sequestration of CO<sub>2</sub> in Low Rank Coals; Velenje Basin, Slovenia as a Natural Analogue  
Dr. Tjaša Kanduč
14. Pharmaceutical and Personal Care Product Residues in the Environment: Occurrence, Sources, Treatment and Effects  
Prof. Ester Heath
15. Petrology of Brown (Low-rank) Coals as Mined and/or Used in Slovenia, Natural Gasses in Them, and Their Gas-sorption Properties  
Dr. Tjaša Kanduč
16. Comparative Study of Ecosystem Management and Services in Contrasting Slovenian Freshwater Systems  
Dr. David Kocman
17. Carbon Dynamics in Forest Soils and the Rhizosphere  
Prof. Nives Ogrinc
18. In-situ Remediation of Polluted Grounds in the Area of the Zinc-works in Celje  
Prof. Janez Ščančar
19. The Use of Specific Methods for Determination and Prevention of Adulteration of Milk and Dairy products  
Prof. Nives Ogrinc
20. 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 Fishermen)  
Prof. Vekoslava Stibilj
21. Evaluation of Quality and Safety Parameters of Vegetables Produced on Different Systems in Slovenia and Abroad with Aim to Establish National Quality Scheme for Vegetables  
Prof. Nives Ogrinc
22. Geomicrobial Factors influencing Mercury Transformations in Transition Zone of Middle and South Adriatic Sea  
Dr. Arne Bratkič
23. EMRP - PartEmission; Emerging Requirements for Measuring Pollutants from Automotive Exhaust Emissions  
Prof. Milena Horvat
24. EMRP; Traceable Measurements for Monitoring Critical Pollutants under the European Water Framework Directive (WFD-2000/60/EC)  
Prof. Radmila Milačič

## RESEARCH PROGRAMS

1. Cycling of Substances in the Environment, Mass Balances, Modelling of Environmental Processes and Risk Assessment  
Prof. Milena Horvat
2. Modelling and Environmental Impact Assessment of Processes and Energy Technologies  
Prof. Borut Smodiš

## R & D GRANTS AND CONTRACTS

1. Synthesis, Characterisation and Use of Novel Ruthenium Compounds in Electrochemotherapy of Tumors (Basic Research Project)  
Prof. Janez Ščančar
2. Toxic Metals and Organometallic Compounds in the Terrestrial Environment  
Prof. Radmila Milačič
3. Speciation and Interactions of Chemical Contaminants at Trace Level in Aqueous Media to Support the Development of Cost-effective Removal Technologies  
Prof. Milena Horvat
4. Development of Molecularly Imprinted Polymers and their application in environmental and bio-analysis  
Asst. Prof. Tina Kosjek
5. Sustainable Land Use in Relation to Soil and Crop Quality  
Prof. Nives Ogrinc
6. Metagenomics for Bioexploration and Biomining of Bacterial Laccases for a Sustainable

## NEW CONTRACTS

1. Radiological Analysis of Groundwater, Soil and Rocks in the Main Researches of the Geosphere and Hydrosphere in Light of Construction of the LILW Repository  
Prof. Vekoslava Stibilj  
National Laboratory of Health, Environment and Food
2. Sustainability Appraisal of Energy Policy Development in Slovenia by 2030 with the Emphasis on Nuclear Option  
Asst. Prof. Branko Kostič  
Gen energija, d. o. o.
3. Evaluating Geological Sequestration of CO<sub>2</sub> in Low Rank Coals; Velenje Basin, Slovenia as a Natural Analogue  
Dr. Tjaša Kanduč  
Velenje Coal Mine
4. Monitoring of the Radioactivity in the Environment in Republic of Slovenia for the Years 2013-2014 - PART 2  
Prof. Vekoslava Stibilj  
Ministry of Agriculture, Forestry and Food
5. Operational and Immission Monitoring in the NEK Surrounding in 2014 and 2015  
Dr. Marko Štok  
Krško Nuclear Power Plant
6. Monitoring of the Radioactivity in Drinking Water for the year 2014  
Prof. Vekoslava Stibilj  
Ministry of Health
7. Technical Support in the Permitting Processes for Seveso Lower Tier Establishments in

- Slovenia  
Asst. Prof. Branko Koutić  
Ministry of Agriculture, Forestry and Food
8. Analysis of Tributyl and Dibutyltin Compounds in Slovene Marine Environment in the Year 2014  
Dr. Tea Zuliani  
Ministry of Agriculture, Forestry and Food
9. Technical Guidelines for Industrial Accidents Risk Prevention in the Phase of Spatial Plan Preparation for the Business Zone Litoštroj P-ZIN-9/14  
Dr. Davor Koutić  
The City of Ljubljana
10. Human Biomonitoring - Chemical Analysis of Metals  
Prof. Milena Horvat  
Ministry of Health

## VISITORS FROM ABROAD

- Ilya Samoiloov, Institute of Radiation Safety and Ecology, National Nuclear Centre of the Republic of Kazakhstan, Kurchatov, Kazakhstan, 11 January–14 February 2014
- Osama Mhmood Hamed Ahmed, Sudan Atomic Energy Commission (SAEC), Ministry of Science and Technology, Khartoum, Sudan, 27 January–27 May 2014
- Fabio Paolo Polo, Università Ca' Foscari, Dorsoduro, Venice, Italy, 1 February–1 August 2014
- Maja Dimitrovska, Arsova Sarafinovska, Anita Najednkoska, Institute for Public Health of the Republic of Macedonia, Skopje, Republic of Macedonia, 24–28 March 2014
- Christiana Odumah Anderson, University of Cape Coast, Department of Physics, Cape Coast, Ghana, 26 April–22 October 2014
- Dr. Maria Ângela de Barros Correia Menezes, CDTN/CNEN – Centro de Desenvolvimento da Tecnologia Nuclear, Belo Horizonte, Minas Gerais, Brazil, 14–30 May 2014
- Misato Ohno, Hokkaido University, Sapporo, Japan, 9 August–21 September 2014
- Dr. Ryoko Fujiyoshi, Hokkaido University, Sapporo, Japan, 7–16 September 2014
- Giada Zanuttini, University of Udine, Udine, Italy, 15 October–22 December 2014
- Dr. Frederica Camin, Trento, Italy, 12 June 2014
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- Ryusuke Imura, Hitoshi Kodamatani, Kagoshima University, Faculty of Science, Japan, 9–16 June 2014
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## MENTORING

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5. Breda Novotnik, *The use of stable chromium isotopes in speciation analysis and investigation of transformation of chromium species in environmental samples*: doctoral dissertation, Ljubljana, 2014 (mentor Radmila Milačič; co-mentor Janez Ščančar).
6. Matej Sedlar, *Temperature fractionation of mercury in solid samples*: doctoral dissertation, Ljubljana, 2014 (mentor Milena Horvat).
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9. Jerneja Planinc, *Genotypic and phenotypic characterization of *Bacillus subtilis* riverbank isolates*: master's thesis, Ljubljana, 2014 (mentor Ines Mandič-Mulec; co-mentor Nives Ogrinc).





# 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 robotics (including intelligent control, humanoids, cognitive robotics, robot learning and vision), automation, biocybernetics, ergonomics and environmental physiology. The common theme of our research endeavours to date has been optimising “the behaviour of man and machine”, accounting for interactions with the environment. Recently, we have added “human-robot partnership” as an additional goal of our research programme. By combining engineering sciences and life sciences, we have been able to make significant contributions to the development of: 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 “Automation, robotics and biocybernetics” in the field of Production Technologies (leader prof. dr. Igor B. Mekjavic). Members of the department participate in several EU projects in the area of cognitive systems, robotics and space technologies. We are also active in transferring our research results into various applications through direct collaboration with industry. By maintaining a critical mass of researchers in all areas within one programme group, we have managed to foster exciting multidisciplinary projects.*



Head:  
Asst. Prof. Aleš Ude

During the past year, the main research topics in the department included humanoid and cognitive robotics, intelligent control of robot systems and contact modelling, robot learning, robot vision, robotic assistive devices, the automation of industrial manufacturing, studies of human physiology in extreme environments, an evaluation of protective equipment, and the development of biomedical methods.

## Robotics

Research in the area of humanoid and cognitive robotics as well as robot learning is primarily conducted within the Humanoid and Cognitive Robotics Lab, which operates within the department. The aim of this laboratory is to create robots capable of helping people and interacting with them in natural environments.

In 2014 we continued our successful collaboration in the FP7 integrated project Xperience (Robots bootstrapped through learning from experience, <http://www.xperience.org/>). The goal of Xperience is to demonstrate that state-of-the-art cognitive robotic systems can be significantly extended by using the concept of structural bootstrapping to generate new knowledge. This process is founded on explorative knowledge acquisition, and subsequently validated through experience-based generalization. In the past year we focused on bootstrapping mechanisms that enable faster motor learning by exploration. The proposed approach enables the robot to exploit existing knowledge, which is given in the form of a database of motor patterns, to direct the search for related motor patterns. In this way the robot can quickly acquire new example movements, which are added to the database to increase the motor knowledge and decrease the need for a lengthy random search for new solutions. Another problem that we addressed is the reuse of motor knowledge gained in one task for learning the appropriate motor behaviour in another task. The proposed methodology exploits a new extension of the concept of dynamic movement primitives (DMPs). We were able to reuse existing motor knowledge when optimizing the speed profiles of new movements.

**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. The common denominator in robotics and biomedical research is improving the quality of life.**



Figure 1: Human-robot cooperative task execution.

**We developed a new concept for imitation learning that enables the consideration of forces and torques arising during the execution of the task in physical contact with the environment. In 2014 we extended the proposed methodology to dual-arm mechanisms. Dual-arm manipulation is considered to be one of the most important features for the new generation of industrial robots.**

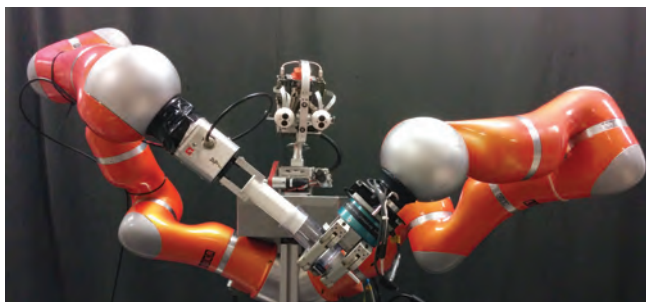


Figure 2: Dual-arm assembly of a cake-decoration tool.

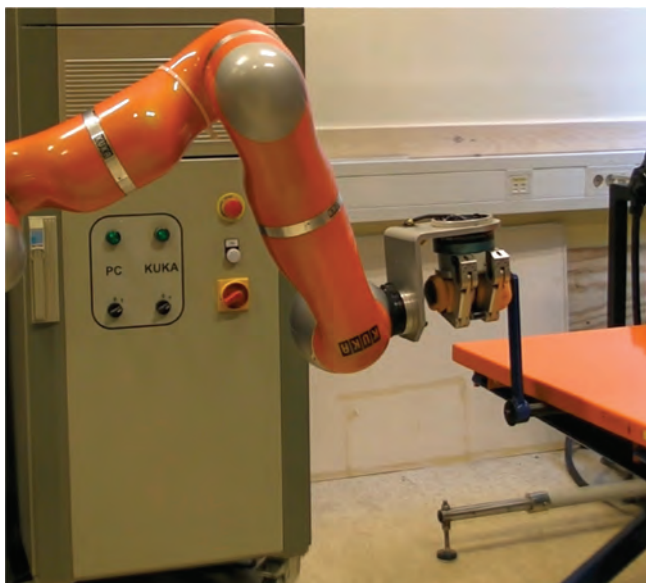


Figure 3: Compliant execution of periodic motion for crank turning without mathematical task models.

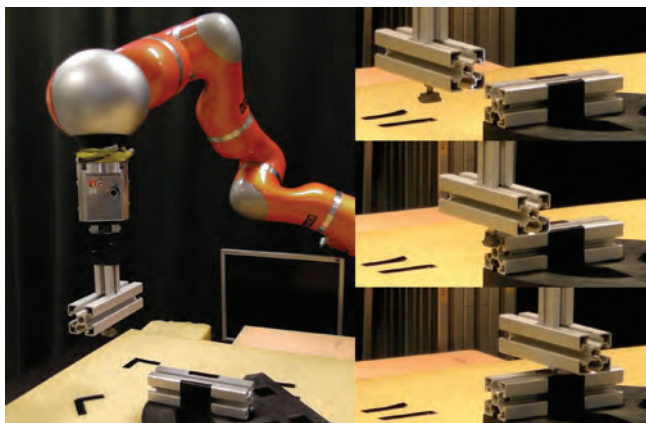


Figure 4: Robot arm while performing a part-assembly task using a human-in-the-loop learning approach.

On the algorithmic level, we improved the speed of explorative learning for coupled DMPs by combining mechanisms such as feedback-error learning and iterative learning control.

Another focus in the Xperience project was the development of a new coaching system, where a human coach interactively changes the robot's motion to achieve the desired outcome. To determine human intentions in terms of coaching, visual as well as haptic information is used. The robot is able to switch between force- or vision-based coaching, depending on the forces applied on the robot's TCP and the current configuration of the human hand. With the proposed coaching system a human teacher can effectively alter the existing robot skill knowledge.

In the past year we successfully completed the FP7 project IntellAct (Intelligent observation and execution of Actions and manipulations, <http://intellact.eu/>). In this project we showed that human action knowledge can be transferred to an anthropomorphic robot, not by copying the movements of the human, but by transferring the human action on different levels. Our most important result in this project was the development of a general approach for the learning of force-based skills. It consists of the following stages: 1. acquire a reference trajectory and the associated force-torque profile that successfully solves the task in a specific workspace configuration by kinesthetic guiding; 2. refine the acquired trajectory and the associated force-torque profile to improve the task dynamics; 3. transfer the acquired skill to new task contexts using 3-D vision and adapt the resulting motion to the trained force-torque pattern. In collaboration with an industrial partner we transferred this methodology to an industrial controller. The proposed approach was also extended to a dual-arm robotic system.

Cognitive robots operating in natural environments should be able to quickly acquire new skills without extensive programming and mathematical modelling. In the FP7 project ACAT (Learning and execution of action categories, <http://www.acat-project.eu/>) we investigated the problem of learning task-specific dynamics to enable compliant task execution. The proposed approach is based on executing the initial movements obtained by kinesthetic guiding with different control-gains regimes. In this way we obtain data for the learning of feed-forward torque commands, which are used to specify a motor representation called Compliant Movement Primitive (CMP). The applicability of the proposed approach was shown on discrete (weight transfer) and periodic tasks (weight lifting and crank turning). However, the learned CMPs are task-specific and need to change if the task context is changed. To mitigate this problem, we applied statistical learning techniques in order to obtain the appropriate CMPs for previously unexplored task variations inside the training space. With this addition, the robot is able to learn and perform variations of the (semantically) same task in a compliant manner without the need for experts to program the movements and time-consuming training processes.

Besides developing new computational learning technologies, our department is also interested in developing new interfaces to support motor learning. In 2014 we continued to advance our previous approaches for transferring human motor skills to the robot with the ability to teach the robot how to compliantly interact with humans and the environment. Our approach rests on the idea of including the human cognitive and sensorimotor capabilities into the robot control loop. We taught an industrial robot how to solve various part-assembly tasks where the robot needs to constantly adapt the compliance of its end-effector. For this purpose we built a novel hand-held impedance control interface that allowed the tutor to modulate the robot's compliance based on the given task requirements.

In the scope of the FP7 project CoDyCo (Whole-body compliant dynamical contacts in cognitive humanoids, <http://www.codyco.eu/>) we studied



how humans utilize hand contacts while executing a whole-body task. We developed a novel experimental paradigm that gave us an insight into the mechanisms of human motor control through continuous mild perturbations that did not provoke reactive arm movements found in similar studies. We measured various biomechanical parameters. The analysis revealed that the contribution of the lower leg muscles was significantly reduced when the subjects were able to use the additional hand support. On the other hand, the activation of trunk flexors was higher when the subjects used the additional hand support and the activation of the trunk extensors remained unchanged. Based on this biomechanical study, we are now constructing a mathematical model that will allow the transfer of our findings to robotics.

In the field of biomechanics our department participated in the project “The influence of the ski’s width to the safety of alpine skiing”, which was successfully completed in 2014. Our most important result in this project is a new procedure for determining the skier’s pose. We developed a new algorithm based on adaptive linear local models (LWPR), which estimates the skier’s pose based solely on a sequence of positions of the antenna, mounted behind the skier’s neck. This trajectory was captured using a high-precision GNSS device. In the study we compared the novel LWPR-based algorithm with other approaches and confirmed the advantages of the proposed method. The main benefit of the proposed approach is a simplified and more accurate measurement of the skier’s kinematics and dynamics using GNSS.

In the area of assistive robotics we designed an exoskeleton control method for the adaptive learning of assistive joint torque profiles in periodic tasks. We used human muscle activity as the feedback to adapt the assistive joint torque behaviour in a way that the wearer’s muscle activity is minimised. The wearer can then relax, while the exoskeleton takes over the task execution. The main advantage of our method compared to other methods is that it does not require any modeling of the wearer’s body. We experimentally evaluated our approach where subjects wearing an arm exoskeleton had to move an object of an unknown mass according to a predefined reference motion. This study was carried out in collaboration with ATR Computational Neuroscience Laboratories, Kyoto, Japan.

We have been conducting research in the area of advanced robot control in unstructured environments for many years. As in such environments unexpected contacts between the robot and an object can occur, it is necessary that the robot system can detect obstacles in real time and also to react after contacts. For the robots equipped with joint torque sensors, we proposed a method for the estimation of the contact forces acting anywhere on the body of the robot. Based on the measured joint torques and the known dynamic model of the robot, the contact point and force are calculated. By using an appropriate control strategy for exploiting the kinematic redundancy of the robot system, the robot can move away from the obstacle causing the contact force or it can change the compliance at the contact point to reduce the redundancy and decrease the contact force.

#### Automation and industrial robotics

An important mission of our department is to transfer our research results to industrial applications. In previous years we carried out a number of projects for the glass industry, including the development of a system for automated glass-forming operations. By performing these projects, we acquired specific knowledge about glass-production technologies and a deeper understanding of the processes involved. We identified a number of operations where a change in technology is needed or would be beneficial. Based on this, we defined and proposed a number of national and international projects, aimed out investigating robot solutions or the generally automated solutions of glass-industry operations. We also collaborated with an R&D department of a national food company, setting down an operating plan and achieving an agreement, under which we will conceive, design and develop a supervision and control system for the automation of a larger food-item production plant. The project will be carried out in the coming year.

In 2014 we also prepared a framework for the automation of car-lamp production. The main goal is to exploit the possibilities of human-robot cooperation in the field of hybrid assembly for better production quality

**We developed a novel experimental paradigm that gave us an insight into the mechanisms of human motor control through continuous mild perturbations that did not provoke reactive arm movements found in similar studies. We are now constructing a mathematical model that will allow the transfer of our findings to robotics.**



Figure 5: Biomechanical study of human motor control

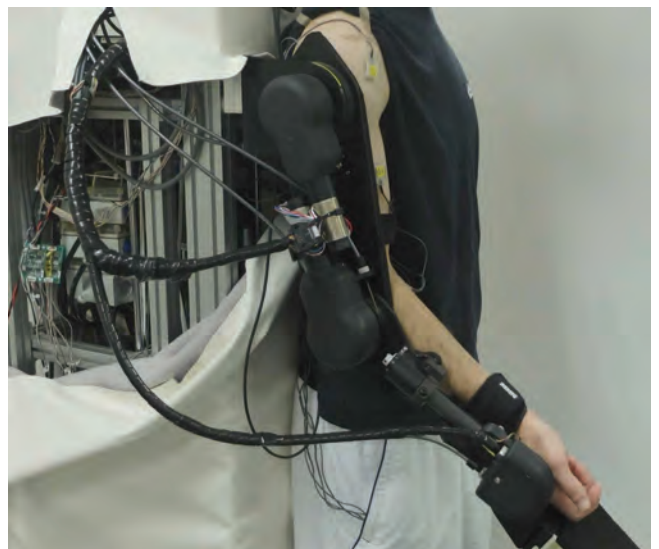


Figure 6: Subject wearing the arm exoskeleton used to evaluate the developed adaptive control method (collaboration with ATR, Japan).





Figure 7: Within the framework of a project supported by ESA we tested the Equivalent Air Altitude Theory at the Antarctic Research Station Concordia.

and to decrease the production costs. As the handling and assembly in car-lamp production are complex tasks, we have proposed achieving the automation and robotization in several steps. In the first step, cooperating robots will be implemented for two tasks: the fastening of coolers and PCBs and their assembly in a housing, and the final packaging of the lamps into the transport carton.

#### Environmental physiology and ergonomics

The Biocybernetics group in our department focuses primarily on research projects concerning the influence of extreme environmental factors on humans as well as the development and evaluation of technology, and strategies to maintain safety and unhindered performance in such extreme environments.

We investigate the effect of a simulated planetary habitat environment on different human physiological systems (<http://www.planhab.com>). For technical reasons, the environment within future Lunar and Mars habitats will be hypobaric and hypoxic. Prolonged exposure to low gravity results in a deconditioning of vital physiological systems, and may consequently constitute a threat to the health of the astronauts. However, it is not known

how prolonged exposure to both reduced gravity and hypoxia will affect health. For the purpose of this research program we established a Planetary Habitat Simulation Facility at the Olympic Sport Centre Planica. Male and female subjects participated in three trials: hypoxic and normoxic bedrest and hypoxic ambulation. The effects of these interventions were investigated in experiments concerning metabolic, cardiorespiratory, musculoskeletal, haematological, immunological and thermoregulatory functions. We anticipate that the new knowledge gained

from these studies will also have clinical implications, since chronic hypoxia and bedrest (inactivity/unloading) constitutes a model of the underlying chronic condition experienced by patients suffering from respiratory insufficiency, cardiac diseases and obesity.

The purpose of our hypoxic exercise confinement study was to investigate the additive effects of exercise training during continuous hypoxic exposure on different physiological systems with special reference to appetite regulation, oxidative stress and sleep modulation. Our project was based on recent evidence suggesting that hypoxia *per se* and in combination with exercise influences appetite and body-mass modulation and could therefore

provide a viable strategy for inducing weight loss and also for treating different metabolic disorders. This is one of the key priorities of modern research in the field of non-communicable disease prevention, given the fact that the prevalence of obesity is escalating in the modern world. The obtained results indicate that exercise does not significantly influence hormonal appetite regulation or sleep quality during hypoxic confinement. However, we showed that exercise significantly blunts oxidative stress and therefore seems to be beneficial for an individual's wellbeing during high-altitude sojourns.

Our research on the comparison of the effects of normobaric and hypobaric hypoxia, partly supported by the European Space Agency, examines the acute and chronic effects of living at altitude on several physiological mechanisms: i) central sleep apnea, ii) nocturnal vasodilatation, iii) sleep architecture, and iv) aetiology of acute mountain sickness. The results obtained in normobaric hypoxia at the Olympic Sport Centre Planica have been compared with the results obtained during exposure to hypobaric hypoxia. The latter were obtained on staff at the Concordia Antarctic Research Station, and members of the Elbrus 2014 expedition. With regards to the physiological responses monitored, these studies have confirmed the Equivalent Air Altitude Theory. Namely, that it is the partial pressure of oxygen that is the main factor influencing the responses monitored, and not the ambient pressure.

Despite a plethora of cross-sectional data on foot size in different age periods there is an obvious lack of data regarding longitudinal foot development during childhood. The aim of our project on foot growth kinetics in children, which was undertaken jointly with an industrial partner (UCS), is to obtain high-quality longitudinal data on foot growth during the childhood

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**We established a research program, funded in part by the European Space Agency (ESA) Programme for European Cooperating States (PECS), the EC FP7 programme, and the Slovenian Research Agency, investigating the separate and combined effects of hypoxia and sustained inactivity/unloading (bedrest) on human physiological systems.**

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Figure 8: Evaluating autonomic characteristics of human temperature regulation.

developmental period. During the course of the two-year project we measured the length, width, and height of the feet of 850 children between the ages of 1 and 15 years, at three-month intervals, using a foot scanner developed by UCS. The project will provide the data necessary to develop an algorithm of foot growth in children, which will be implemented in a web-based system advising parents on appropriate footwear for their children.

This project evaluated the regional thermal comfort in males and females. The subjects were requested to regulate the temperature of the water delivered to a water-perfused suit, such that it was thermally comfortable. In separate trials, subjects regulated the temperature of the whole suit, or specific regions of the suit covering different skin areas (arms, legs, front torso, back torso, hands, feet, and head). In the absence of regulation, the temperature changed in a sinusoidal manner from 10°C to 50°C; by depressing a switch, and reversing the direction of the temperature at the limits of the thermal comfort zone (TCZ), each subject defined the TCZ for each body segment that was investigated.

We continue our development of thermal manikins by embedding their control systems with physiological algorithms for simulating the onset and gain of sweating based on the core and shell temperatures. Together with our partner, the University of Maribor, we have developed a whole-body manikin with such capabilities. This work was funded by the Slovene Research Agency. We are currently developing a thermoregulatory head manikin with such functionality, for the evaluation of helmets.

Within the framework of the Marie Curie IRSES grant “International cooperation for the advancement of research on the underlying systems of human thermoregulation”, we initiated a research collaboration with the University of Cape Town on thermoregulatory adaptations to heat. The aim of the project was to advance the current understanding of physiological responses to thermal stress and the main underlying mechanisms. One of our researchers spent a year as a post-doctoral fellow at the University of Cape Town, investigating different aspects of heat acclimation and performance in the heat. We also examined the effect of seasonal variation on the characteristics of behavioural and autonomic temperature regulation.

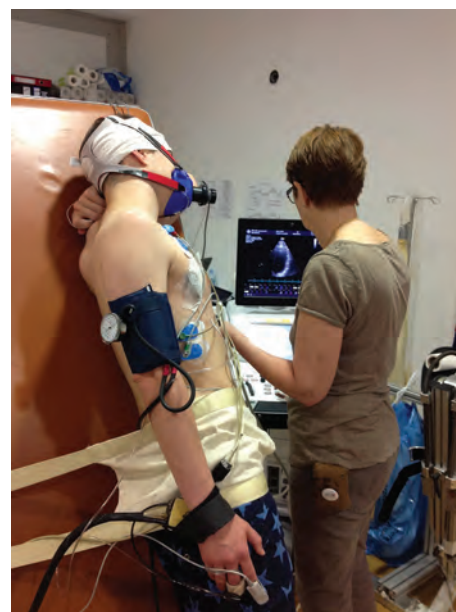


Figure 9: Measurement of cardiovascular responses during an orthostatic tolerance test.

### Some outstanding publications in the past year

1. Gams, A., Nemec, B., Ijspeert, A. J., Ude, A.: Coupling movement primitives: Interaction with the environment and bimanual tasks. *IEEE Transactions on Robotics*, 2014, vol. 30, no. 4, 816–830
2. Babič, J., Petrič, T., Peternel, L., Šarabon, N.: Effects of supportive hand contact on reactive postural control during support perturbations. *Gait & posture*, 2014, vol. 40, no. 3, 441–446
3. Nemec, B., Petrič, T., Babič, J., Supej, M.: Estimation of alpine skier posture using machine learning techniques. *Sensors*, 2014, vol. 14, no. 10, 18898–18914
4. Debevec, T., McDonnell, A., MacDonald, I., Eiken, O., Mekjavić, I. B.: Whole body and regional body composition changes following 10-day hypoxic confinement and unloading/inactivity. *Applied physiology, nutrition and metabolism*, 2014, vol. 39, no. 3, 386–394.
5. McDonnell, A., Eiken, O., Jaki, P., Mekjavić, I. B.: Circadian rhythm of peripheral perfusion during 10-day hypoxic confinement and bed rest. *European journal of applied physiology*, 2014, vol. 114, no. 10, 2093–2104

### Awards and appointments

1. A. Gams and T. Petrič: Best Scientific Paper Award at 23rd International Conference on Robotics in Alpe-Adria-Danube Region, Smolenice, Slovakia, 2014
2. Tadej Debevec: Top three in Hypoxia and Mountain Medicine with article "Does Moderate Exercise Alter Hormonal Appetite Regulation and Oxidative Stress during Continuous Hypoxic Exposure?"

### Organization of conferences, congresses and meetings

1. Review meeting of EU project Xperience, Ljubljana, Slovenia, 14–16 April 2014
2. Advances in Robot Kinematics - 14th International Symposium, Ljubljana, 29 June–3 July 2014
3. General meeting of EU project CoDyCo, Ljubljana, Slovenia, 20–21 October 2014

## INTERNATIONAL PROJECTS

1. Stimulators and Parts  
Asst. Prof. Aleš Ude  
Foreign buyers
2. Development of Curved LCD Shutter  
Asst. Prof. Leon Žlajpah  
Kimberly-Clark
3. 7FP - ICARUS; International Cooperation for the Advancement of Researcher on the Undelaying System of Human Thermoregulation  
Prof. Igor Mekjavić  
European Commission

4. 7FP - Xperience; Robots Bootstrapped through Learning from Experience  
Asst. Prof. Aleš Ude  
European Commission
5. 7FP - IntellAct; Intelligent Observation and Execution of Actions and Manipulation  
Asst. Prof. Aleš Ude  
European Commission
6. 7FP - PlanHab; Planetary Habitat Simulation  
Asst. Prof. Igor Kovač  
European Commission
7. 7FP - ACAT; Learning and Execution of Action Categories  
Asst. Prof. Aleš Ude  
European Commission
8. 7FP - CoDyCo; Whole-body Compliant Dynamical Contacts in Cognitive Humanoids  
Asst. Prof. Jan Babič  
European Commission
9. Accelerated Development of Autonomous Behaviors for Humanoid Robots  
Asst. Prof. Aleš Ude  
Slovenian Research Agency
10. Advanced Perception and Learning for Heterogeneous Cognitive Robots  
Asst. Prof. Bojan Nemeč  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Avtomation, Robotics and Biocybernetics  
Prof. Igor Mekjavič

## R & D GRANTS AND CONTRACTS

1. Dual Nature of Stem Cells in Cancer and their Application in Therapy  
Prof. Igor Mekjavič
2. Learning, Analysis, and Detection of Motion in the Framework of a Hierarchical Compositional Visual Architecture  
Asst. Prof. Aleš Ude
3. The Role of Small GTPases in the Regulation of Endosomal/Lysosomal Transport in Astrocytes  
Prof. Igor Mekjavič
4. The Detection of Irregularities and Fraud in the Financing of the Public Health Services  
Dr. Marjeta Kramar Fijavž
5. Methods of Algebra and Functional Analysis in Theory and Practice of Financial Mathematics  
Prof. Igor Klep
6. 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 Mekjavič
7. Hypoxic Inactivity: Implications for Heart Failure, Respiratory Insufficiency and Obesitas  
Prof. Igor Mekjavič
8. Influence of Ski Width on Alpine Skiing Safety  
Asst. Prof. Bojan Nemeč

## NEW CONTRACT

1. Monitoring Foot Growth in Children  
Prof. Igor Mekjavič  
UCS, Kupcu prilagojeni proizvodi, d. o. o.

## VISITORS FROM ABROAD

1. Dr. Fares Abu-Dakka, University of Madrid, Spain, 15 – 25 June 2014
2. Craig Asmundsen, Simon Fraser University, Canada, 29 May – 6 June 2014
3. Dr. Morteza Azad, University of Birmingham, United Kingdom, 20– 22 October 2014
4. Prof. Tamim Asfour, University of Karlsruhe, Germany, 11 – 16 April 2014
5. Marwan Bel Guedbad, University Paris Sud, France, 2 June – 1 September 2014
6. Prof. Branislav Borovac, University of Kragujevac, Faculty of Technical Science, Serbia, 6 – 9 October 2014
7. Laura Calisesi, University of Bologna, Italy, 1 October – 31 December 2014
8. Jean-Luc Cordel, Kimberly-Clark Professional, USA, 29 September 2014
9. Jens Skov Damagaard, Aalborg University, Denmark, 15 September – 5 October 2014
10. Dr. Helio Fernandez, University of Brussels, Belgium, 21 – 25 July 2014
11. Dr. Charles Fuller, University of San Diego, USA, 21 – 24 August 2014
12. Prof. Paolo Gallina, University of Trieste, Italy, 27 November 2014
13. Dr. Mikael Grönkvist, Royal Institute of Technology, Sweden, 20 November– 14 December 2014
14. Dr. Martina Heer, DLR, Germany, 21 – 24 August 2014
15. Prof. Fatma Kalaouglu, Istanbul Technical University, Turkey, 18 December 2014
16. Dr. Michail Keramidias, Royal Institute of Technology, Sweden, 1 – 30 November 2014
17. Kelly Kolb, Kimberly- Clark Professional, USA, 29 September 2014
18. Dr. Stylianos Kounalakis, Evelpidon University, Greece, 1 – 22 November 2014
19. David Lilley, Kimberly-Clark Professional, USA, 12 March 2014
20. Prof. Chris Miall, University of Birmingham, United Kingdom, 20 – 21 October 2014
21. Dr. Dragomir Nenchev, Laboratory na Musashi Institute of Technology, Japan, 11 September 2014
22. Prof. Francesco Nori, Italian Institute of Technology, Italy, 20 – 21 October 2014
23. Prof. Vincent Padois, University of Pierre and Marie Curie, France, 20 – 21 October 2014
24. Prof. Vincenzo Parenti Castelli, University of Bologna, Italy, 24 February 2014
25. Prof. Petar Petrovič, Faculty of Mechanical Engineering, Serbia, 6 – 9 October 2014
26. Asst. Prof. Mirko Raković, Faculty of Technical Science, Serbia, 6– 9 October 2014
27. Prof. Aleksandar Rodić, Institute Mihailo Pupin, Serbia, 6– 9 October 2014
28. Elmar Rückert, TU Darmstadt, Austria, 18– 22 August 2014, 17– 22 December 2014
29. Mark Newton, University of Portsmouth, United Kingdom, 28 – 29 May 2014
30. David Schiebener, University of Karlsruhe, Germany, 1– 23 April 2014
31. Bryan Semkuley, Kimberly- Clark Professional, USA, 29 September 2014
32. Prof. Michael M. Stanisic, University of Notre Dame, USA, 16 June– 18 August 2014
33. Dr. Nektarios Stavrou, ASPETAR Hospital, Qatar, 27–28 November 2014
34. Prof. Rüdiger Dillmann, Karlsruhe Institute of Technology, Germany, 13. – 16. April 2014
35. Prof. Mark Steedman, University of Edinburgh, UK, 14. – 16. April 2014
36. Prof. Florentin Wörgötter, University of Göttingen, Nemčija, 14. – 16. April 2014
37. Prof. Norbert Krüger, University of Southern Denmark, Danska, 14. – 16. April 2014
38. Prof. Justus Piater, University of Innsbruck, Avstrija, 14. – 16. April 2014
39. Prof. Giorgio Metta, Italian Institute of Technology, Italija, 14. – 16. April 2014

## STAFF

### Researchers

1. Asst. Prof. Jan Babič
  2. Dr. Andrej Gams
  3. Asst. Prof. Igor Kovač
  4. Prof. Igor Mekjavič
  5. Asst. Prof. Bojan Nemeč
  6. Prof. Matjaž Omladič\*
  7. Asst. Prof. Dušan Ponikvar\*
  8. Dr. Anton Ružič
  9. Asst. Prof. Aleš Ude, Head
  10. Asst. Prof. Leon Žlajpah
- Postdoctoral associates
11. Dr. Tarsi Bali, left 01. 07. 14
  12. Dr. Janez Bernik\*
  13. Dr. Kristijan Cafuta\*

14. Asst. Prof. Gregor Cigler\*, left 01. 08. 14
  15. Dr. Tadej Debevec
  16. Dr. Rok Erman\*
  17. Dr. Denis Forte
  18. Prof. Igor Klep
  19. Prof. Tomaž Košir\*
  20. Asst. Prof. Marjeta Kramar Fijavž\*
  21. Dr. Tadej Petrič
  22. Dr. Gregor Šega\*
  23. Dr. Klemen Šivic\*
  24. Dr. Dejan Velušček\*, left 01. 08. 14
- Postgraduates
25. Robert Bevec, B. Sc.
  26. Jernej Čamerlik, B. Sc.
  27. Miha Deniša, B. Sc.



28. Aljaž Kramberger, B. Sc.
29. Nejc Likar, B. Sc.
30. Adam Mc Donnell, B. Sc., left 01. 10. 14
31. Rok Okorn, B. Sc.
32. Luka Peternel, B. Sc.
33. Dr. Barry Martin Ridge
34. Rok Vuga, B. Sc.
- Technical officers
35. Damjan Fink
36. Roman Hribar, B. Sc., left 01. 11. 14

37. Borut Lenart, B. Sc., retired 29. 12. 14
38. Bogomir Vrhovc, B. Sc.
- Technical and administrative staff
39. Tanja Dragojević, B. Sc.
40. Dušan Filipič, retired 31. 12. 14
41. Marija Kavčič, B. Sc.
42. Jana Stanič

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

1. Fares Abu Dakka, Bojan Nemeč, Aljaž Kramberger, Anders Glent Buch, Norbert Krüger, Aleš Ude, "Solving peg-in-hole tasks by human demonstration and exception strategies", *Ind. rob.*, vol. 41, no. 6, pp. 575-584, 2014.
2. Wolfgang Arendt, Dominik Dier, Marjeta Kramar Fijavž, "Diffusion in networks with time-dependent transmission conditions", *Appl. math. optim.*, vol. 69, no. 2, pp. 315-336, 2014.
3. Jan Babič, Tadej Petrič, Luka Peternel, Nejc Šarabon, "Effects of supportive hand contact on reactive postural control during support perturbations", *Gait posture*, vol. 40, no. 3, pp. 441-446, 2014.
4. Gregor Cigler, Marjan Jerman, "On separation of eigenvalues by certain matrix subgroups", *Linear algebra appl.*, vol. 440, pp. 213-217, 2014.
5. Gregor Cigler, Marjan Jerman, "On the separation of eigenvalues by the permutation group", *Special matrices*, vol. 2, iss. 1, pp. 61-67, 2014.
6. Tadej Debevec, Tarsi C. Bali, Elizabeth J. Simpson, Ian A. MacDonald, Ola Eiken, Igor B. Mekjavić, "Separate and combined effects of 21-day bed rest and hypoxic confinement on body composition", *Eur. j. appl. physiol.*, vol. 114, no. 11, pp. 2411-2425, 2014.
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8. Tadej Debevec, Vincent Pialoux, Igor B. Mekjavić, Ola Eiken, Pauline Mury, Grégoire P. Millet, "Moderate exercise blunts oxidative stress induced by normobaric hypoxic confinement", *Med. sci. sports exerc.*, vol. 46, no. 1, pp. 33-41, 2014.
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13. Norbert Krüger et al. (15 authors), "Technologies for the fast set-up of automated assembly processes", *KI, Künstl. Intell. (Oldenbourg)*, vol. 28, no. 4, pp. 305-313, 2014.
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16. Ljilja Milanković, Martin Zorko, Jan Babič, Bojan Nemeč, Matej Supej, "3D gibanje kolenskega sklepa pri manipulaciji prijemališča sile reakcije podlage v medio-lateralni smeri: pilotska študija simulacije alpskega smučanja", *Šport (Ljublj.)*, vol. 62, no. 1/2, pp. 76-80, 2014.
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18. Shawnna A. Morrison, Jurij Gorjanc, Igor B. Mekjavić, "Mount Everest and Makalu cold injury amputation", *High alt. med. biol.*, vol. 15, no. 1, pp. 78-83, 2014.
19. Bojan Nemeč, Tadej Petrič, Jan Babič, Matej Supej, "Estimation of alpine skier posture using machine learning techniques", *Sensors*, vol. 14, no. 10, pp. 18898-18914, 2014.
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21. Tadej Petrič, Leon Žlajpah, Gianluca Garofalo, Christian Ott, "Walking with adaptive oscillator and dynamic movement primitives", In: Special issue of the JOMaC dedicated to the 21st edition of the Workshop on Robotics in Alpe-Adria-Danube Region, RAAD 2013, Portorož, Slovenia, *Int. j. mech. control*, vol. 15, no. 1, pp. 3-9, 2014.
22. Tadeja Režen, Anja Kovanda, Ola Eiken, Igor B. Mekjavić, Boris Rogelj, "Expression changes in human skeletal muscle miRNAs following 10 days of bed rest in young healthy males", *Acta physiologica*, vol. 210, no. 3, pp. 655-666, 2014.
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24. Aleš Ude, "Estimation of Cartesian space robot trajectories using unit quaternion space", *Int. j. adv. robot. syst.*, vol. 11, pp. 137-1-137-8, 2014.

## REVIEW ARTICLE

1. Ola Eiken, Igor B. Mekjavić, Roger Kölegård, "Blood pressure regulation In: in vivo mechanical properties of precapillary vessels as affected by long-term pressure loading and unloading: [invited talk]", *Eur. j. appl. physiol.*, vol. 114, no. 3, pp. 499-509, 2014.

## SHORT ARTICLE

1. Tadej Debevec, Grégoire P. Millet, "Discerning normobaric and hypobaric hypoxia: significance of exposure duration", *J Appl Physiol*, vol. 116, no. 9, pp. 1255, 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Morteza Azad, Jan Babič, Michael N. Mistry, "Effects of hand contact on the stability of a planar humanoid with a momentum based controller", In: *HUMANOIDS 2014, IEEE-RAS 14th International Conference on Humanoid Robots*, November 18th-20th, 2014, Madrid, Spain, Danvers, IEEE, 2014, pp. 348-353.
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  12. Nejc Likar, Leon Žlajpah, "Estimation of contact information using nonlinear optimization", In: *Conference proceedings*, 23rd International Workshop on Robotics in Alpe-Adria-Danube Region [also] RAAD 2014, September 3 - 5, 2014, Smolenice, Slovakia, Danvers, IEEE =Institute of Electrical and Electronics Engineers, 2014, 6 pp.
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  22. Rok Vuga, Bojan Nemeč, Aleš Ude, "Speed profile optimization through directed explorative learning", In: *HUMANOIDS 2014*, IEEE-RAS 14th International Conference on Humanoid Robots, November 18th-20th, 2014, Madrid, Spain, Danvers, IEEE, 2014, pp. 547-553.
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Andrej Gams, Bojan Nemeč, Tadej Petrič, Aleš Ude, "Coupling of trajectories for human-robot cooperative tasks", In: *Advances in robot kinematics*, Jadran Lenarčič, ed., Oussama Khatib, ed., Cham [etc.], Springer, cop. 2014, pp. 537-544.
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## MENTORING

1. Barry Ridge, *Learning basic object affordances in a robotic system*: doctoral dissertation, Ljubljana, 2014 (mentor Aleš Leonardis; co-mentor Danijel Škočaj).
2. Anja Barle, : master's thesis, Ljubljana, 2014 (mentor Dejan Velušček).
3. Domen Butala, : master's thesis, Ljubljana, 2014 (mentor Dejan Velušček; co-mentors Gregor Papa, Sabrina Guettes).
4. Nace Čebulj, : master's thesis, Ljubljana, 2014 (mentor Matjaž Omladič; co-mentor Gregor Šega).

*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 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 2014 was devoted to three sub-areas: methodologies for analysis and control systems design; tools and building blocks for implementation; and applied research in the priority problem domains.

The sub-area *methodologies for analysis and control systems design* included three topics.

The first topic addressed the *modelling and identification of nonlinear and complex dynamical systems*.

The research in the dynamic system modelling of Gaussian process models was directed towards the modelling of biological and environmental systems and control design based on the models. Part of the research was devoted to an alternative method, which was the modelling of dynamic systems with model-tree ensembles. A key feature of modern condition monitoring systems is the ability to predict the remaining useful life of the system or its components. To achieve this, the work on the topic of development of condition monitoring and the prediction of the remaining useful life of the system or its components continued with the development of new computational procedures that combine the sequential Monte-Carlo approach with a classical Kalman filter. The results of the work are two specifically designed algorithms for an estimation of the remaining lifetime of electrochemical energy systems, i.e., Li-ion batteries and PEM fuel-cell systems.

The second topic was *advanced control*. We have continued the work on improvements to the cascade scheme of magnetic plasma control for the Iter fusion tokamak reactor. A prototype MPC controller for the ITER plasma current and a shape controller were designed in order to assess the feasibility of its practical real-time implementation, and its control performance in the suppression of specific disturbances and in regulation near constraints was compared to a scheme based on singular perturbation decomposition.

The third topic of interest was *condition monitoring and fault diagnosis*. The emphasis in this area has been on new procedures for triggering alarms based on a feature analysis. It is an urgent problem, because in practice changes often take place in features that are not caused by injury, but due to disturbances and changes in the working conditions of the system. As a consequence, undesirable false alarms can frequently be actuated. To prevent this we have developed a robust process which – unlike the previously known processes – does not over-react to changes of the features value, but to the change of the shape of its distribution function. The “differences” between the latter and the shape in its nominal state in the presence of damage are expressed through the generalized Jensen-Renyi divergence. The procedure was successfully demonstrated for a number of experimental data obtained on bearings (Figure 1). The main feature is that its settings need a minimal amount of a priori information and that it also works successfully, even in the presence of non-measurable changes in the operating conditions. For the originality of the algorithm we received a special award at the International Conference

CMMNO. Another interesting result is a solution to the problem of the detection of changes in the components of the spectrum. The basis for the solution is an effective approximation of the distribution function of the spectral component using the weighted distribution  $\chi^2$ . In 2014 we also continued our work on the diagnostics of PEM fuel cells with use of impedance measurements. Based on the previous research findings, we developed a new diagnostic approach, which is based on a statistical analysis (Figure 2). The output of the approach is a condition indicator that has a direct relation to the possible faults in the PEM fuel cells. The main benefit of the approach is its ability to give results without any previous characterization measurement, which are undesirable in industrial systems. The results of this work were presented in two journal papers published in the *Journal of Power Sources*.



Head:

**Dr. Vladimír Jovan**

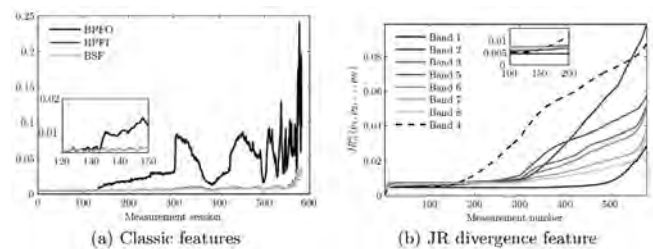


Figure 1: Comparison between the time evolution of the classical features related to bearing faults (left) and the generalised Jensen-Renyi divergence.

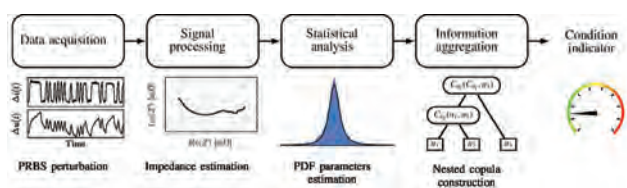


Figure 2: Schematic representation of the complete condition-monitoring process for a fuel-cell stack

In the area **tools and building blocks for the implementation**, the MAGICCS methodology for the development and automatic generation of process control software has been further developed. An important part of the development environment, i.e., the ProcGraph model editor, was developed in recent years. In 2014 the development of a system for the automatic mapping of ProcGraph models into the code of the industrial controllers was in progress. At the same time, in the frame of the “Research Voucher” project, an adaptation and implementation of the methodology

was continuing for a Slovenian engineering company. In 2014 we have also continued with the development of a software prototype called ProOpter, which enables the analysis of production dynamics. The commercial potential of such a tool was evaluated together with the development of a business model. Our product idea (ProOpter) was chosen as one of top-ten selected “early-stage” innovations to be presented at the Heidelberg Innovation Forum 2014 (early-stage innovations).

**Applied research in the priority problem domains** was the third sub-area of our interest.

In 2014 we delivered a new final-product end-quality assessment system to Domel d.o.o. (Figure 3), the main producer of motors for vacuum cleaners in the EU. The system is fully integrated into a new, centralised reporting and configuration system. The complete setup and data analysis is now performed using an internal web-based application. Additionally, we developed a platform for the endurance testing of EC motors, together with the accompanying controller units. Both systems are designed following the MIMOSA OSA-EAI standard.

*Control of wastewater treatment plants* is our next traditional research area. We participated in an improvement to the aeration control at the Ljubljana Wastewater Treatment Plant (Ljubljana WWTP). Several changes were made to the existing aeration control. The parameters of the common air rail pressure controller were adjusted and the air-pressure set-point controller and the airflow controller were introduced. With the improved aeration control, savings of up to 10 % in the electrical consumption are being achieved on a yearly basis.

#### International and national R&D projects

In the frame of three-year international project Eurostar *ProDisMon-Probabilistic Distributed Industrial System Monitor* we developed, in collaboration with the partner INEA, a test rig for validating the diagnostic and prognostic algorithms for industrial applications. Since practical usage is much conditioned on a clear economic benefit, we suggested an approach to the validation of maintenance strategies relying on a stochastic model of the degradation processes in machine components.

In 2014 the FW7 project *FCGEN-Development and on-truck demonstration of diesel-powered FC-based power unit* was in its 3rd year. In this period the complete fuel processor has been assembled and tested. In November



Figure 3: Diagnostic system for total quality control in the new production line of eco-motors at Domel

2014 our group has also taken over the coordination of the FCGEN project from Volvo. On the technical side our group has successfully implemented the developed control system and further optimized it (Figure 4). Besides that, the DCDC power converter and dedicated APU ECU have been developed. The former has already been tested, while for the latter, the software development is in final stages.

The aim of the next FW7 project *FluMaBack- Fluid Management component improvement for back up fuel cell systems* is the development and optimization of the balance-of-plant components of a fuel-cell system. The activities in 2014 include: analysis of the mechanical fault modes of the air blower and an analysis of the durability of the electrical components of the underlying controller. The results allowed the proper set up of the end-quality control line as well as a proposal for upgrading the controller, thereby enhancing its durability.

From April 2014 we also participated in the third FW7 project *Diamond-Diagnosis-aided control for SOFC power systems*. The objective of the project is to improve the performance and lifetime of solid-oxide fuel-cell (SOFC) systems, by developing advanced controls and diagnosis tools that

provide meaningful information about the actual state-of-the-health of the entire system. Our activities carried out in the first year of the project were related to the design of low-level controllers for system units and a soft sensor for an estimation of the maximum and minimum fuel-cell stack temperatures.

In collaboration with the consortium ENEA/CREATE from Naples, Italy, in 2014 we have successfully applied a 3-year project “Fast Model Predictive Control for Magnetic Plasma Control - FMPC/FMPC” to the “Enabling Research” call of the EUROfusion Work Programme 2015 (part of Horizon 2020 / Euratom). The aim of the project



is to apply novel, fast MPC approaches to plasma magnetic control, where MPC is currently not applicable due to the large-scale multivariable nature of the problem and sub-second sampling rates.

Within the scope of the Slovenian Research Agency's applicative project "*Optimisation of the refrigeration energy costs in shopping centres*" in 2014 an approach was developed to evaluate defrosting needs. The approach measured the refrigerator temperatures and accordingly estimates the accumulated frost. For a cost optimisation the structure of the physical model has been determined. The developed model describes the temperature dynamics of the refrigerator and the food.

The aim of another ongoing Slovenian Research Agency applicative project "*Development and implementation of methods for real-time modelling and forecasting air pollution*" is to develop a methodology and Gaussian-processes-based model to predict the ozone concentration above the selected, most congested, locations in Slovenia. Data from the Nova Gorica (Figure 5) and Bilje monitoring stations were used for the analysis, where we have identified the regressors with the greatest influence on the daily forecast of the ozone concentration. The data are prepared to validate the methods for the on-line learning of time-varying models, which are being developed within the project.

In 2014 we completed two projects for industrial partners and signed a new contract (with Danfoss Trata). In Domel d.o.o. we installed a new diagnostic system for the electromotors of type 458, which performs the final quality control on the production line. The system is positioned as the last stop in the production of electric motors and provides the real-time detection of errors in the produced suction units. To the Danfoss Trata d.o.o. company we delivered an electronic module and firmware software for "heavy-duty" drives valves.

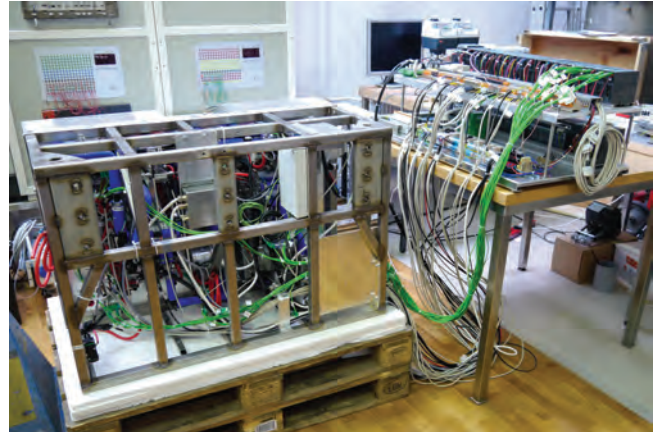


Figure 4: Testing of a fuel reformer's connections with the controller

#### Educational and training activities

Some members of the department are giving lectures and practical courses at different faculties and universities: the Faculty of Electrical Engineering, University of Ljubljana, the Faculty of Logistics, University of Maribor, the University of Nova Gorica and the "Jožef Stefan" International Postgraduate School. They also act as supervisors of Ph.D. students.

#### Some outstanding publications in the past year

1. Debenjak, A., Boškosi, P., Musizza, B., Petrovčič, J., Juričić, D.: Fast measurement of proton exchange membrane fuel cell impedance based on pseudo-random binary sequence perturbation signals and continuous wavelet transform. *Journal of power sources*, ISSN 0378-7753, vol. 254, 112–118
2. Boškosi, P., Debenjak, A.: Optimal selection of proton exchange membrane fuel cell condition monitoring thresholds. *Journal of power sources*, ISSN 0378-7753, vol. 268, 692–699
3. Pregelj, B., Vrečko, D., Petrovčič, J., Jovan, V., Dolanc, G.: A model-based approach to battery selection for truck onboard fuel cell-based APU in an anti-idling application. *Applied energy*, ISSN 0306-2619, vol. 137, 64–76
4. Dolanc, G., Belavič, D., Hrovat, M., Hočevar, S., Pohar, A., Petrovčič, J., Musizza, B.: A miniature fuel reformer system for portable power sources. *Journal of power sources*, ISSN 0378-7753, Dec. 2014, vol. 271, 392–400
5. Leamy, D., Kocijan, J., Domijan, K., Duffin, J., Roche, R. A. P., Commins, S., Collins, R., Ward, T. E.: An exploration of EEG features during recovery following stroke - implications for BCI-mediated neurorehabilitation therapy. *Journal of neuro-engineering and rehabilitation*, ISSN 1743-0003, 2014, vol. 11, no. 9, 1–16

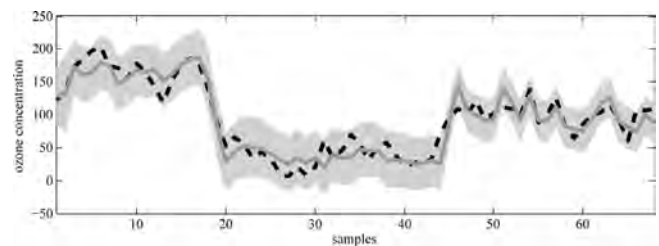


Figure 5: Daily forecast of ozone concentrations with a GP model (Nova Gorica)

#### Some outstanding achievements in the past year

1. The development and implementation of a diagnostic system for the final quality control of electric motors in Domel d.o.o. The installed system is the eighth such system for the automatic final control of electric motors for vacuum cleaners used by Domel, which covers over 60% of the European market and produces over 3 million motors annually.



2. The prototype module ProOpter.IVS had been selected as one of top ten early-stage innovations that were presented at the Heidelberg Innovation Forum 2014 focusing on „*Smart Production and Manufacturing - Innovative ICT Solutions and Production Processes*“. The module selects from the production database the most influential process variables that optimise the production process.
3. Our department members were awarded at CMMNO14 - *4th International Conference on Condition Monitoring of Machinery in Non-stationary Operations* with the *Award for an original approach to solving the problem*. The authors Boštjan Dolenc, Pavle Boškovski and Đani Juričić presented an original approach to faults diagnostics in mechanical drives by observing changes in the statistical patterns of distributions functions, i.e., the envelope distribution obtained from vibrations.
4. Our department member, Prof. Juš Kocijan, co-authored the Dictionary of Automatic Control, Systems and Robotics, released by ZRC Publisher. The dictionary contains 1,753 Slovene entries in the field of mathematical modelling, simulation of dynamic systems, automatic control and associated building blocks and robotics.
5. The „Jožef Stefan“ Institute and the Danfoss Trata d.o.o. company have developed a family of intelligent valve drives. This innovative system was nominated for the H&V Award, the biggest award in the UK commercial market for HVAC systems.

### Awards and appointments

1. Boštjan Dolenc was awarded with the PCT Technology Network award (Process Control Technology) for his Master's thesis entitled "Diagnostics of distributed and localized bearing faults"
2. Boštjan Dolenc was awarded for the best Diploma Thesis at Slovenian state competition on maintenance in 2014 at the 24th Slovenian Trade Fair and Conference on Technical Maintenance
3. Boštjan Dolenc was awarded for his original contribution at the 4th International Conference on Condition Monitoring of Machinery in Non-stationary Operations, CMMNO14

## INTERNATIONAL PROJECTS

1. 7FP - FLUMABACK; Fluid Management Component Improvement for Back Up Fuel Cell Systems  
Dr. Pavle Boškovski  
European Commission
2. 7FP - FCGEN; Fuel Cell Based On-board Power Generation  
Dr. Boštjan Pregelj  
European Commission
3. 7FP - DIAMOND; Diagnosis-aided Control for SOFC Power System  
Prof. Đani Juričić  
European Commission
4. COST IC0806, IntelliCIS; Intelligent Monitoring, Control, and Security of Critical Infrastructure Systems  
Dr. Nadja Hvala  
COST Office
5. COST ES1202; Water\_2020: Conceiving Wastewater Treatment in 2020 - Energetic, Environmental and Economic Challenges  
Dr. Darko Vrečko  
COST Office

## RESEARCH PROGRAM

1. Program Systems and Control  
Prof. Đani Juričić

## R & D GRANTS AND CONTRACTS

1. Prognostics and Health Management of Mechanical Drives Based on Novel MEMS Sensor Networks  
Prof. Đani Juričić
2. Development and Implementation of a Method for On-line Modelling and Forecasting of Air Pollution  
Prof. Juš Kocijan
3. Optimisation of Energy Cost for Refrigeration Systems in Shopping Malls  
Asst. Prof. Damir Vrančič
4. Competence Centre for Advanced Control Technologies: CC ACT  
Asst. Prof. Damir Vrančič
5. Probasensor: EUROSTARS; Probabilistic Bayesian Soft Sensor - A Tool for On-line Estimation of the Key Process Variable in Cold Rolling Mills  
Prof. Đani Juričić

## NEW CONTRACTS

1. Process Control Software Development Methodology  
Giovanni Godena, M. Sc.  
Inea, d. o. o.
2. Optimisation of Energy Cost for Refrigeration Systems in Shopping Malls  
Asst. Prof. Damir Vrančič  
Danfoss Trata, d. o. o.

## VISITOR FROM ABROAD

1. Prof. Jan Cvejn, Department of process Control, Faculty of Electrical Engineering and Informatics, University of Pardubice, Pardubice, Czech Republic, 12-20 June 2014

## STAFF

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1. Dr. Gregor Dolanc
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5. Dr. Nadja Hvala
6. **Dr. Vladimir Jovan, Head**
7. Prof. Đani Juričić
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9. Dr. Bojan Musizza
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17. Dr. Miha Glavan
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22. Boštjan Dolenc, B. Sc.
23. Martin Stepančič, B. Sc.
24. Ales Svetek, M. Sc., *left 01. 03. 14*

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  26. Primož Fajdiga, B. Sc.
- Technical and administrative staff
27. Maja Janežič, B. Sc.
  28. Miroslav Štrubelj

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Pavle Boškoski, Andrej Debenjak, "Optimal selection of proton exchange membrane fuel cell condition monitoring thresholds", *J. power sources*, vol. 268, pp. 692-699, dec. 2014.
2. Pavle Boškoski, Matej Gašperin, Dejan Petelin, Ā ani Juričič, "Bearing fault prognostics using Rényi entropy based features and Gaussian process models", *Mech. syst. signal process.*, 11 pp.
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10. Ivan Madjarov, Juš Kocijan, Alexandra Grancharova, Bogdan Shishedjiev, "Towards a service-based framework for environmental data processing", *Int. j. adv. comput. sci. appl.*, vol. 5, no. 4, pp. 44-51, 2014.
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12. Matija Perne, Matt Covington, Franci Gabrovšek, "Evolution of karst conduit networks in transition from pressurized flow to free-surface flow", *Hydrol. earth syst. sci.*, vol. 18, no. 11, pp. 4617-4633, 2014.
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## PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

1. Darko Belavič, Marko Hrovat, Marina Santo-Zarnik, Kostja Makarovič, Andreja Benčan, Janez Holc, Gregor Dolanc, Primož Fajdiga, Stanko Hočevar, Andrej Pohar, Franci Kovač, Marjan Hodnik, Anton Konda, Boris Jordan, Vlasta Sedlakova, Josef Sikula, Barbara Malič, "An overview of LTCC based ceramic microsystems: from simple pressure sensors to complex chemical reactors", In: *Proceedings, EDS' 14, Electronic Devices and Systems IMAPS CS International Conference 2014, June 25-26, 2014, Brno, Czech Republic*, Ondrej Hegr, ed., Brno, Vysoké učení Technické v Brně, 2014, pp. XVI-XXI.

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7. Dejan Gradišar, Miha Glavan, Damir Vrančič, "Ocenjevanje debeline ledu na hladilnih rebrih zmrzovalnih skrinj v trgovskih centrih", In: *Zbornik triindvajsete mednarodne Elektrotehniške in računalniške*

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## MENTORING

1. Darko Aleksovski, *Tree ensembles for discrete-time modeling of non-linear dynamic systems*: doctoral dissertation, Ljubljana, 2014 (mentor Sašo Džeroski; co-mentor Juš Kocijan).
2. Miha Glavan, *Production control using identified models of production performance indicators*: doctoral dissertation, Ljubljana, 2014 (mentor Gašper Mušič).
3. Dejan Petelin, *Approximation methods for modelling dynamic systems with Gaussian processes*: doctoral dissertation, Ljubljana, 2014 (mentor Juš Kocijan).
4. Marko Hančič, *Evaluation of methods for finding the most influential input variables to predict the levels of ozone in the air*: master's thesis, Ljubljana, 2014 (mentor Igor Škrjanc; co-mentor Juš Kocijan).
5. Lea Manfreda, *Modeling and forecasting traffic intensity at road intersections*: master's thesis, Nova Gorica, 2014 (mentor Juš Kocijan).

# ARTIFICIAL INTELLIGENCE LABORATORY

E-3

*The Artificial Intelligence Laboratory (<http://ailab.ijs.si/>) is concerned mainly with the research and development of information technologies, with an emphasis on artificial intelligence. The main research areas are the following: data analysis with an emphasis on text, web and cross-modal data, scalable real-time data analysis, machine learning, the analysis and modelling of large networks, the 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 and presented at international events, they have also developed several software tools for multimodal data analysis. These tools include: Text-Garden, a suite of text-mining tools; OntoGen (<http://ontogen.ijs.si/>), a tool for ontology learning; Document-Atlas (<http://docatlas.ijs.si/>), a tool for complex visualization; Atlas of Slovenian Science (<http://scienceatlas.ijs.si/>), a web portal for analyzing the scientific community; 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; OntoPlus, a methodology for semi-automatic ontology extension; Contextify (<http://contextify.net/>), a tool for contextualized e-mail and contact management; NewsFeed (<http://newsfeed.ijs.si/>), a clean, continuous, real-time aggregated stream of semantically enriched news articles from RSS-enabled sites across the world; iDiversiNews (<http://aidemo.ijs.si/diversinews/>) a system for the processing and visualization of news; Event registry (<http://eventregistry.org/>) a system for identifying mentioned world events in news; Twitter Observatory (<http://twitterobservatory.net/>) a system for the analysis of selected tweets. The laboratory's strategy is to combine scientific excellence and strong industrial collaboration and to transfer research results into real-world business environments.*



Head:  
Prof. Dunja Mladenic

In the past 12 years, members of the Artificial Intelligence Laboratory successfully completed 38 EU projects, of which 5 were concluded in 2014. In addition, we were involved in another 11 EU projects in 2014, including 1 Network of Excellence. In 2014, we were involved in 12 national projects, of which 8 ended in 2014. This includes two Centers of Competence and one Research Voucher, two applied research projects and one basic research project. In addition, we have successfully concluded two industrial projects, one with the Slovenian press Agency and the other with the University of Ljubljana. Together with the Department for Communication Systems in collaboration with Adria Mobil, we have developed sensor technologies and artificial intelligence methods for the user-friendly and energy-efficient functioning of an auto-home that is being tested in a real-world environment.

In the area of statistical data modelling and machine learning we have contributed a "Big Data Tutorial" at the Large Scale Online Learning and Decision Making Workshop - LSOLDM 2014 (Marko Grobelnik, Blaž Fortuna, Dunja Mladenic). In the EU FP7 project *XLike (Cross-lingual Knowledge Extraction)* coordinated by our department, we have developed technology for the real-time detection and extraction of events from multilingual news streams. This technology was integrated into a prototype Event Registry (<http://eventregistry.org/>), which was validated by Bloomberg and the Slovenian Press Agency, where it provides discovery and analysis support to the editorial team and financial analysts. In the EU FP7 project TOPOSYS (Topological Complex Systems), coordinated by our department, we have made significant progress in understanding the underlying mathematical foundations of multi-scale dynamic systems, in particular using topological tools. More efficient algorithms have been developed to understand the dynamics of complex systems, along with a more thorough understanding of the statistical behaviour of computed invariants as well as generalizing

**Dunja Mladenic had an invited talk "Semantic Search for Complex Data" at the Council of Europe.**



Figure 1: Event Registry a system for cross-lingual news analysis and identification of the mentioned world events.



the invariants themselves beyond functions. In particular, we developed tight bounds on the maximal statistics of noise as well as established central limit theorems for these algebraic objects, both of which are the first results of their kind. In the EU FP7 project *Symphony (Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy)* our work is mainly focused on developing tools and approaches for nowcasting based on media monitoring. We have established a social media monitoring data infrastructure, connecting social media data from Twitter with news events from the Event Registry system. We have also been working on an analysis

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**Jure Leskovec, an associated member of our department from Stanford University, received the award Zois Ambassador of Science of the Republic of Slovenia.**

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of opinion diffusion to be used later in nowcasting macroeconomic indicators.

In the areas of **text and network analysis** and **language technologies**, we have contributed two invited talks on “Global Media Monitoring” at the Brazilian Machine Learning and Knowledge Discovery in Databases School (<http://www.amda.icmc.usp.br/mlkdd2014/>) and at the ESWC Summer School on Semantic technologies 2014 (Marko Grobelnik). We have organized a workshop “Data Science for News Publishing” at the international conference KDD 2014 (<http://ailab.ijs.si/~blazf/NewsKDD2014/>). We have contributed a presentation on “Cross-lingual Data Analysis” at the University of Zagreb. In 2014, the first funding was received from the Slovenian Research Agency for setting up the Slovenian CLARIN infrastructure. The European research infrastructure CLARIN serves researchers from the fields of humanities and social sciences. Its goal is to facilitate researchers in these fields with access to language resources, technologies and expertise. The Slovenian research infrastructure CLARIN.SI is organised as a consortium of partners. The CLARIN.SI platform currently collects freely available concordances and other tools and services for working with the Slovene language, while the repository of language resources is in the construction phase. The JSI also participated in a project funded by the Ministry of Culture dedicated to topics on language policy for Slovene. It is a four-year project; the portal is in the construction phase. When opened, it will include information on legal aspects of language rights, links to online language resources, tools, services

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**Marko Grobelnik had an invited talk “Global Media Monitoring” at the Council of Europe.**

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and technologies, information about language-learning possibilities and an online consultation service about frequent language problems. In EU FP7 project *Sophocles (Self-Organised information Processing, Criticality and Emergence in multilevel Systems)*, we have been working on processing social media data (Twitter, newspaper archive, event streams) with the goal of validating the theoretical models developed in the project. We studied the emergence of scales in the news streams and worked on the validation of hierarchical models. We also focused on the social network of Twitter users with the goal of finding the tipping point (or critical) behaviour of the network.

In the area of **semantic technologies**, we contributed two invited talks at “Search in Parliaments” (<http://assembly.coe.int/nw/Conferences/Search-in-Parliaments/Seminar-Programme-EN.asp>), one on Semantic Search for Complex Data (Dunja Mladenič) and the other on Global Media Monitoring (Marko Grobelnik). We have concluded the EU FP7 Network of Excellence *Planet Data (Intelligent Information Management)*, where we have contributed methods for detecting events in the ‘Smart City’ context and techniques for cleaning and repairing sensor data. In EU FP7 project *ProaSense (The Proactive Sensing Enterprise)* we have developed tools for the visualization of sensor data in the production process. The project is one of the early adopters of a shift from reactive to proactive computing. The FP7 EU project *XLime (Cross-Lingua, cross-Media knowledge extraction)* is dedicated to fusing the knowledge from different dimensions of media content, providing a near real-time, continuously updated and comprehensive view on knowledge diffusion across media. We have developed methods for the analysis

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**Together with the Centre for Knowledge Transfer in Information Technologies, following the success of videoLectures.NET, recognized by the UN and UNESCO as one of the most outstanding examples of creative and innovative e-Content in the world in the past decade, the “Jožef Stefan” Institute has successfully established a UNESCO Chair on Open Technologies for Open Educational Resources and Open Learning. The Chair is currently expanding its vision and strategy in collaboration within OpeningupSlovenia and with the Knowledge 4 All Foundation Ltd based in London, UK.**

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of information derived from various media channels, such as audio, video, text and social media as a first step towards the development of a real-time comprehensive view on knowledge diffusion across media and languages.

**Knowledge management** includes research and development using methods and tools from a broader Artificial Intelligence area in real business settings. The aim of the FP7 EU project *NRG4Cast (Energy Forecasting)* coordinated by our department, is the development of real-time management, analytics and forecasting services for energy-distribution networks in urban/rural communities. Our work is focused on analysing multimodal data streams from the energy domain. We have developed analytical methods for data cleaning and fusion integrating them into an analytic platform. In NRG4Cast, we introduced an innovative framework to combine various analytical techniques (from data mining to reasoning) in one modular solution, which provides valuable results to various stakeholders in the business chain. In the FP7 EU project, *MobiS (Personalized Mobility Services for energy*

*efficiency and security through advanced Artificial Intelligence techniques*) we have developed services for traffic-data collection, cleaning and fusion that are used by the traffic-prediction services. A part of this is a novel approach to the short-term traffic prediction of various parameters, including traffic flow, speed and occupancy for several prediction horizons. We have developed a simple reasoning engine UMKO that is used as an efficient alternative to Cyc, helping operators in the traffic call centre (AMZS). All these services together serve as a traffic platform, which is currently used by the call-centre expert system and custom mobile application prototype (Mobis Commuting Assistant) with the idea being to help the daily commuters on their travels. We have concluded the FP7 EU project *Mediamixer (Community set-up and networking for the remixing of online media fragments)* on the use of fragmented media content. In collaboration with the Department for Communication Systems (E6), we have started work on a new EU FP7 project *SunSeed*, where our contribution is focused on short-term load forecasting for smart electricity distribution.

**Promotion of science** is continually present in the efforts of the Artificial Intelligence Laboratory. Marko Grobelnik had an interview on Media Data Analytics for the newspaper "Finance". Dunja Mladenić had an interview on Artificial Intelligence and Robotics (<http://www.jana.si/2014/10/zlovesce-napovedi-o-koncu-clovestva/>). Mitja Jermol had an interview on national television on Open Education Technology (<http://4d.rtvlo.si/#arhiv/voli-in-izvoli/174278670>, <http://www.rtvlo.si/slovenija/odprto-izobrazevanje-slovenija-zeli-voditi-pot-v-inovativnost-in-povezovanje/335280>). In collaboration with the Centre for Knowledge Transfer in Information Technologies (CT3) we have successfully concluded the EU FP7 project *TransLectures (Transcription and Translation of Video Lectures)*, where we have developed innovative tools for the automatic transcription and translation of educational video material. Together with CT3, we continued to use the *videlectures.NET* portal to promote artificial intelligence, the Jožef Stefan Institute and Slovenian research in general. Our laboratory is also among the main organizers and supporters of the annual national ACM Computer Science Competition for secondary-school students; in 2014 more than 150 students participated in the competition. We have been organizing a touring exhibition about female PhD holders from the area of computer science in Slovenia since 2006, thereby promoting the role of women in science (<http://ScienceWithArt.ijs.si/>).

In 2014, we were very actively involved in submitting new project proposals, particularly within the H2020 Programme. Once again, we were very successful, obtaining funding for three new projects in H2020: European Data Science Academy (EDSA), Aquasmart and OPTIMUM. We continue with our successful efforts to include Slovenian industry into the European research area, where over the past 10 years we have produced a list of 18 companies participating in EU projects.

## Some outstanding publications in the past year

1. Leskovec, J., Rajaraman, A., Ullman, J. D.: *Mining of massive datasets*. 2nd ed. Cambridge: Cambridge University Press, 2014. XI, 467 pages
2. Tomašev, N., Radovanović, M., Mladenić, D., Ivanović, M.: The role of Hubness in clustering high-dimensional data. *IEEE transactions on knowledge and data engineering*, ISSN 1041-4347. [Print ed.], 2014, vol. 26:3, 739–751
3. Škraba, P., Wang, B.: Interpreting feature tracking through the lens of robustness. In: BREMER, Peer-Timo (ed.). *Topological methods in data analysis and visualization III : theory, algorithms applications : [presented at TopoInVis 2013, March 4-6, 2013, Davis, USA]*, (Mathematics and visualization). Cham: Springer, 2014, 19–37
4. McAuley, J. J., Leskovec, J.: Discovering social circles in ego networks. *ACM transactions on knowledge discovery from data*, ISSN 1556-4681, 2014, vol. 8:1, 4-1-4-28
5. Rehm, G., Grobelnik, M., Krek, S., et al.: The strategic impact of META-NET on the regional, national and international level : a large-scale evaluation. In Ninth International Conference on Language Resources and Evaluation, May 26-31, 2014, Reykjavik, Iceland. CALZOLARI, Nicoletta (ed.). *LREC 2014 : proceedings*. [S. l.]: ELRA, 2014, 1517–1524

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## INTERNATIONAL PROJECTS

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| 1. 7FP - SiS CATALYST; Children as Change Agents for the Future of Science in Society<br>Prof. Dunja Mladenić<br>European Commission | Prof. Dunja Mladenić<br>European Commission   |
| 2. 7FP - PlanetData<br>Marko Grobelnik<br>European Commission  | 4. 7FP - X-Like; Cross-lingual Knowledge Extraction<br>Marko Grobelnik<br>European Commission |
| 3. 7FP - LT-Web; Language Technology in the Web  | 5. 7FP - transLectures; Transcription and Translation of Video Lectures                       |

- Prof. Dunja Mladenić  
European Commission
6. 7FP - TOPOSYS; Topological Complex System  
Dr. Primož Škraba  
European Commission
  7. 7FP - NRG4CAST; Energy Forecasting  
Maja Škrjanc, B. Sc.  
European Commission
  8. 7FP - MobiS: Personalized Mobility Services for Energy Efficiency and Security through Advanced Artificial Intelligence Techniques  
Marko Grobelnik  
European Commission
  9. 7FP - Sophocles; Self-Organised Information Processing, Criticality and Emergence in Multilevel Systems  
Marko Grobelnik  
European Commission
  10. 7FP - MEDIAMIXER; Community Set-up and Networking for the Remixing of Online Media Fragments  
Marko Grobelnik  
European Commission
  11. 7FP - xLiMe; CrossLingual CrossMedia Knowledge Extraction  
Marko Grobelnik  
European Commission
  12. 7FP - SYMPHONY; Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy  
Prof. Dunja Mladenić  
European Commission
  13. 7FP - ProaSense; The Proactive Sensing Enterprise  
Marko Grobelnik  
European Commission
  14. 7FP - SUNSEED; Sustainable and Robust Networking for Smart Electricity Distribution  
Prof. Dunja Mladenić  
European Commission
  15. 7FP - FI-IMPACT; Future Internet Impact Assurance  
Marko Grobelnik  
European Commission
  16. PARSEME: PARSing and Multi-Word Expressions. Towards Linguistic Precision and Computational Efficiency in Natural Language Processing.  
Dr. Simon Krek  
COST Office
  17. IS1305, European Network of E-Lexicography (ENEL)  
Dr. Simon Krek  
COST Office
  18. Dynamic Network Analysis of Global News Events  
Prof. Dunja Mladenić  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Knowledge Technologies  
Prof. Dunja Mladenić

## R & D GRANTS AND CONTRACTS

1. Information-Communication Technologies and Transformation of Survey Research in Social Sciences  
Marko Grobelnik
2. Model for Domain-Specific Trend Prediction based on Semantic Enrichment of Unstructured Patterns  
Prof. Dunja Mladenić
3. Development and Evaluation Automation of Survey Questionnaire  
Marko Grobelnik
4. Quality of Service and Quality of Experience Measurement and Control System in Multimedia Communications Environments  
Marko Grobelnik
5. Co-authorship Networks of Slovenian Scholars: Theoretical Analysis and Visualization User Interface Development  
Prof. Dunja Mladenić
6. Open Communication Platform for Service Integration: CC OPCOMM  
Prof. Dunja Mladenić
7. Cloud Assisted Services: CC CLASS  
Marko Grobelnik
8. Topological Machine Learning  
Dr. Primož Škraba

## NEW CONTRACTS

1. Development Project for Establishing a Platform of Advanced Services for Energy Management of Household Consumers  
Marko Grobelnik  
Solvera Lynx, d. d.
2. Technologies for Next-Generation Intelligent Motorhome  
Marko Grobelnik  
Adria Mobil, d. o. o., Novo mesto

## VISITORS FROM ABROAD

1. Flavio Zeni, UNDESA, Kenya, 7–8 January 2014
2. Aleks Jakulin, Ganxy, New York, USA, 4 February 2014
3. Eivind Morgensen, Aker, Fornebu, Norway, 10 March 2014
4. Rudi Studer, FZI, Karlsruhe, Germany, 10 March 2014
5. Nenad Stojanovic, FZI, Karlsruhe, Germany, 10 March 2014
6. Dominik Riemer, FZI, Karlsruhe, Germany, 10 March 2014
7. Babis Magoutas, ICCS, Athens, Greece, 10 March 2014
8. Alexandros Bousdekis, ICCS, Athens, Greece, 10 March 2014
9. Dimitris Apolostou, ICCS, Athens, Greece, 10 March 2014
10. Gregoris Mentzas, ICCS, Athens, Greece, 10 March 2014
11. Aleksandar Stojadinović, NissaTech, Niš, Serbia, 10 March 2014
12. Boban Stajic, NissaTech, Niš, Serbia, 10 March 2014
13. Brian Elvesæter, SINTEF, Trondheim, Norway, 10 March 2014
14. Stig Ole Johnsen, SINTEF, Trondheim, Norway, 10 March 2014
15. Paulo Figueras, UNINOVA, Caparica, Portugal, 10 March 2014
16. Ruben Costa, UNINOVA, Caparica, Portugal, 10 March 2014
17. Ana Rita Campos, UNINOVA, Caparica, Portugal, 10 March 2014
18. John Davies, British Telecom, London, United Kingdom, 26–29 March 2014
19. Abe Hsuan, Hsuan and Irwin LLC, New York, USA, 26–29 March 2014
20. Michael Witbrock, Cypcorp, Austin, USA, 26–29 March 2014
21. James Hodson, Bloomberg, New York, USA, 26–29 March 2014
22. Stefano Pacifico, Bloomberg, New York, USA, 26–29 March 2014
23. Stephane Guerlliot, AFP, Paris, France, 26–29 March 2014
24. Stavros P. Xanthopoulos, Fundação Getulio Vargas of FGV Online, Rio de Janeiro, Brazil, 25–26 April 2014
25. Colin de la Higuera, Université de Nantes, Nantes, France, 25–26 April 2014
26. Geoffrey J. Gordon, Carnegie Mellon University, Pittsburgh, USA, 25–26 April 2014
27. Divina Frau-Meigs, Sorbonne Nouvelle, Paris, France, 25–26 April 2014
28. Dorian Šuc, Vegasoul Capital, Hong Kong, China, 23 May 2014
29. Ruben Sipoš, Cornell University, Ithaca, USA, 11 July 2014
30. Aleks Jakulin, Columbia University, New York, USA, 14 August 2014
31. Rok Sosič, Stanford University, Palo Alto, USA, 41890
32. Jean-Pierre Guglielmi, Council of Europe Parliamentary Assembly, Strasbourg, France, 18–20 September 2014
33. Julien Klaus, Council of Europe Parliamentary Assembly, Strasbourg, France, 18–20 September 2014
34. Erik Gran, Sintef, Trondheim, Norway, 14 August 2014
35. Rimmert van der Kooij, Sintef, Trondheim, Norway, 14 August 2014
36. Estevam Hruschka, Federal University of São Carlos, Sao Carlos, Brazil, 6 October 2014
37. Mauro Gallegati, Univerze Politecnica della Marche, Ancona, Italy, 27–29 October 2014
38. Antonio Palestrini, Univerze Politecnica della Marche, Ancona, Italy, 27–29 October 2014
39. Stefano Pacifico, Bloomberg, New York, USA, 27–31 October 2014
40. Alfons Hoekstra, University of Amsterdam, Amsterdam, Netherlands, 30 November–4 December 2014
41. Rick Quax, University of Amsterdam, Amsterdam, Netherlands, 30 November–4 December 2014
42. Janusz Holyst, University of Warsaw, Warsaw, Poland, 30 November–4 December 2014
43. Anton Golub, Olsen Ltd, Zürich, Switzerland, 30 November–4 December 2014
44. Borja Minano-Maldonado, Universitat de les Illes Balears, Palma, Spain, 1–4 December 2014
45. Joana Masso, Universitat de les Illes Balears, Palma, Spain, 1–4 December 2014
46. Michael Witbrock, Cypcorp, Austin, USA, 14–19 December 2014

## STAFF

### Researchers

1. Dr. Damjan Bojadžiev
  2. Asst. Prof. Branko Kavšek\*
  3. Dr. Gregor Leban
  4. Prof. Dunja Mladenić, Head
  5. Asst. Prof. Iztok Savnik\*
  6. John Stewart Shawe-Taylor, B. Sc.
  7. Dr. Primož Škraba
- ### Postdoctoral associates
8. Dr. Janez Brank
  9. Dr. Blaž Fortuna
  10. Dr. Gregor Jerše\*, left 12. 08. 14
  11. Dr. Aljaž Košmerlj
  12. Dr. Simon Krek
  13. Dr. Jurij Leskovec
  14. Dr. Andrej Muhič\*
  15. Dr. Inna Novalija
  16. Dr. Joao Paulo Pita Da Costa
  17. Dr. Polona Škraba Stanič
  18. Dr. Mikael Vilhelm Vejdemo Johansson, left 01. 07. 14
- ### Postgraduates
19. Luka Bradeško, B. Sc.
  20. Rayid Ghani, M. Sc.
  21. Dejan Govc\*
  22. Mitja Jermol, M. Sc.
  23. Blaž Kazič, B. Sc.

24. Alexandra Moraru, B. Sc.
  25. Blaž Novak, B. Sc.
  26. Jan Rupnik, B. Sc.
  27. Janez Starc, B. Sc.
  28. Luka Stopar, B. Sc.
  29. Tadej Štajner, B. Sc., left 01. 05. 14
  30. Mitja Trampuš, B. Sc., left 01. 04. 14
- ### Technical officers
31. Flavio Fuart, B. Sc.
  32. Zala Herga, B. Sc.
  33. Dr. Ganna Kudryavtseva
  34. Mojca Mikac\*, B. Sc.
  35. Matjaž Rihtar, B. Sc.
  36. Jasna Škerbec, B. Sc., left 01.07.14
  37. Maja Škrjanc, B. Sc.
- ### Technical and administrative staff
38. Evgenia Belyaeva, B. Sc., left 01. 10. 14
  39. Marko Grobelnik
  40. Klemen Kenda
  41. Mojca Kregar Zavrl, B. Sc.
  42. Miha Papler
  43. Mateja Zver, B. Sc.

Note:

\* part-time JSI member

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1. Simon Krek, "Prva in druga izdaja SSKJ", V: *Leksikografija*, vol. 2, no. 2, pp. 114-160, 2014.
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3. Andrej Muhič, Bor Plestenjak, "A method for computing all values  $\lambda$  such that  $A + \lambda B$  has a multiple eigenvalue", *Linear algebra appl.*, vol. 440, pp. 345-359, 2014.
4. Mateja Pirš, Barbara Eržen, Mišo Šabovič, Primož Karner, Ludvik Vidmar, Mario Poljak, Borut Jug, Mojca Mikac, Janez Tomažič, "Early atherosclerosis in HIV-infected patients below the age of 55 years: Slovenian national study", *Wien. Klin. Wochenschr.*, jg. 126, hft. 9/10, pp. 263-269, May 2014.
5. João Pita Costa, "On the coset category of a skew lattice", *Demonstr. Math.*, vol. 47, no. 3, pp. 539-554, 2014.
6. Nenad Tomašev, Miloš Radovanović, Dunja Mladenić, Mirjana Ivanović, "Hubness-based fuzzy measures for high-dimensional k-nearest neighbor classification", *Int. j. mach. learn. cybern.*, vol. 5, no. 3, pp. 445-458, 2014.
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8. Mitja Trampuš, Dunja Mladenić, "Constructing domain tempates with concept hierarchy as background knowledge", *Inf. technol. valdyn.*, vol. 43, no. 4, pp. 414-432, 2014.
2. Tomaž Erjavec, Jan Jona Javoršek, Simon Krek, "Raziskovalna infrastruktura CLARIN.SI", In: *Jezikovne tehnologije: zbornik 17. mednarodne multikonference Informacijska družba - IS 2014, 9. - 10. oktober 2014, [Ljubljana, Slovenia]: zvezek G: proceedings of the 17th International Multiconference Information Society - IS 2014, October 9th - 10th, 2014, Ljubljana, Slovenia: volume G*, Tomaž Erjavec, ed., Jerneja Žganec Gros, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 19-24.
3. Polona Gantar, Iztok Kosem, Simon Krek, "Slovene lexical database: lexicographical process", In: *Workflow of Corpus-based Lexicography*, Bolzano, European Network of e-Lexicography, 2014.
4. Iztok Kosem, Polona Gantar, Nataša Logar, Simon Krek, "Automation of lexicographic work using general and specialized corpora: two case studies", In: *The user in focus: proceedings of the XVI EURALEX International Congress, 15 - 19 July 2014, Bolzano/Bozen*, Andrea Abel, ed., Chiara Vettori, ed., Natascia Ralli, ed., Bolzano, Institute for Specialised Communication and Multilingualism, cop. 2014, pp. 355-364.
5. Aljaž Košmerlj, Jenya Belyaeva, Gregor Leban, Blaž Fortuna, Marko Grobelnik, "Crowdsourcing event extraction", In: *Data science for social good*, KDD 2014, 20th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, August 24-27, new York City, USA, 3 pp..
6. Simon Krek, Polona Gantar, Iztok Kosem, "Razlage v novem slovarju slovenskega jezika", In: *Novi slovar za 21. stoletje: e-zbornik s Posveta o novem slovarju slovenskega jezika na Ministrstvu za kulturo, 12. februar 2014*, Irena Grahek, ed., Simona Bergoč, ed., Ljubljana, Ministrstvo za kulturo, 2014.
7. Nikola Ljubešić, Kaja Dobrovoljc, Simon Krek, Marina Peršurić Antičić, Darja Fišer, "hrMWElex: a MWE lexicon of Croatian extracted from a parsed gigacorpuz", In: *Jezikovne tehnologije: zbornik 17. mednarodne multikonference Informacijska družba - IS 2014, 9. - 10. oktober 2014, [Ljubljana, Slovenia]: zvezek G: proceedings of the 17th International Multiconference Information Society - IS 2014, October 9th - 10th, 2014, Ljubljana, Slovenia: volume G*, Tomaž Erjavec, ed., Jerneja Žganec Gros, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 25-31.

### REVIEW ARTICLE

1. Simon Krek, "Terminologija kot storitev", *Teor. praksa*, vol. 51, no. 4, pp. 670-683, 705, jul.-avg. 2014.

### PUBLISHED CONFERENCE CONTRIBUTION

1. Željko Agić, Jörg Tiedemann, Kaja Dobrovoljc, Simon Krek, Daniela Merkle, Sara Može, "Cross-lingual dependency parsing of related languages with rich morphosyntactic tagsets", In: *Proceedings of the EMNLP'2014 workshop: language technology for closely related languages and language variants: LT4CloseLang 2014, October 29, 2014, Doha, Qatar*, [Stroudsburg], Association for Computational Linguistics, 2014, pp. 13-24.
8. Kiyoshi Nitta, Iztok Savnik, "A distributed query execution method for RDF storage managers", In: *10th International workshop on scalable semantic web knowledge base systems (SSWS 2014)*, (CEUR workshop proceedings, vol. 1261), [S. l.], CEUR-WS, 2014, pp. 45-60.
9. Kiyoshi Nitta, Iztok Savnik, "Survey of RDF storage managers: [Elektronski vir]", In: *Think mind: DBKDA 2014, April 20 - April 24, 2014, Chamonix, France*, Friedrich Laux, ed., et al, 2014, pp. 148-153.



10. Georg Rehm *et al.* (44 authors) , "The strategic impact of META-NET on the regional, national and international level: a large-scale evaluation", In: *LREC 2014: proceedings*, Ninth International Conference on Language Resources and Evaluation, May 26-31, 2014, Reykjavik, Iceland, Nicoletta Calzolari, ed., [S. l.], ELRA, 2014, pp. 1517-1524.
11. Iztok Savič, Kiyoshi Nitta, "Design of distributed storage manager for large-scale RDF graphs: [Elektronski vir]", In: *Think mind: DBKDA 2014, April 20 - April 24, 2014, Chamonix, France*, Friedrich Laux, ed., et al, 2014, pp. 154-160.
12. Primož Škraba, Bei Wang, "Approximating local homology from samples", In: *Proceedings of the Twenty-Fifth Annual ACM-SIAM Symposium on Discrete Algorithms, January 5-7, 2014, Portland, Oregon, USA*, Chandra Chekuri, ed., pp. 174-192.
13. Primož Škraba, Bei Wang, "Interpreting feature tracking through the lens of robustness", In: *Topological methods in data analysis and visualization III: theory, algorithms applications: [presented at TopoInVis 2013, March 4-6, 2013, Davis, USA]*, (Mathematics and visualization), Peer-Timo Bremer, ed., Cham, Springer, 2014, pp. 19-37.
14. Primož Škraba, Bei Wang, Guoming Chen, Paul Rosen, "2D vector field simplification based on robustness", In: *PacificVis 2014, 7th Pacific Visualization Symposium, March 4-7, 2014, Yokohama, Japan, [Piscataway]*, IEEE = Institute of Electrical and Electronics Engineers, 2014, pp. 49-56.

#### PATENT APPLICATION

1. Kiyoshi Nitta, Iztok Savič, *RDF data retrieving apparatus and RDF data retrieving method*, PA2014-129622, Japan Patent Office, 2014.

#### MENTORING

1. Delia Sorina Rusu, *Text annotation using background knowledge: doctoral dissertation*, Ljubljana, 2014 (mentor Dunja Mladenič).

# 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 2014, 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 “COURAGE”, “EmployID” and “REDIRNET”, the “STORK 2.0” and “eSENS” from the CIP (Competitiveness and innovation) programme, and the “D-FET” project from the EU ISEC (Prevention of and Fight Against Crime) programme. 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 Jožef Stefan International Postgraduate School, and the DOBA Faculty. In 2014 they were mentors of four master’s theses and one diploma thesis. One of the main achievements in 2014 was the organisation of the Researchers’ Night in the frame of the “WeForYou” project from Horizon 2020.

### Concepts, architectures, technologies and services in the future internet

The first area of research and development was focused on security infrastructures and trusted services. The Laboratory for Open Systems and Networks is involved in the creation of a Pan-European infrastructure that is needed for secure cross-border services based on national eID credentials, such as digital identity cards. The work is being performed in collaboration with partners from two large-scale pilots from the EU Competitiveness and Innovation Programme (CIP): STORK 2.0 and eSENS.

The main goal of a “Secure identity across borders linked 2.0 (STORK 2.0)” project with 58 partners from 19 European countries is to enable secure e-identity-based services across borders in the fields of e-academia, e-banking, public services for business, and e-health. The project, which will finish in 2015, demonstrated interoperable services in real-life settings and validated common specifications, standards and building blocks, exploring scenarios to address challenging legal and governance issues (across borders, application domains and different sectors) decisively pushing the lines for the wider uptake of eID in Europe. Our main activities in 2014 included the development of the building blocks for a common European infrastructure and the implementation of three e-academia services: virtual learning environment, anonymous electronic survey service, and job-selection service. The services promise to be beneficial for both students and higher educational institutions, as well as for companies that make decisions on the basis of proven academic information, for example, when validating a job applicant’s qualifications in an electronic way.

The “Electronic Simple European Networked Services (eSENS)” project is consolidating the building blocks of several large-scale pilots, including STORK 2.0, focusing strongly on the core building blocks, such as eID, eDocuments, e-Delivery, and e-Signatures. The architecture to be developed will be part of the European Interoperability Architecture (EIA) for the efficient and effective delivery of cross-border and cross-sector electronic public services.

Our laboratory is leading project activities on user-attributes provision and aggregation and role management.

In 2014 we started with the design and development of interoperability solutions for information exchange among the rescue agencies during accidents and other natural disaster situations. Interoperability solutions address the interoperation of the communication networks of different rescue agencies (e.g., police, traffic and road service, medical aid, fire protection agency, general rescue services, mountain-rescue services, anti-terrorism agencies) used for data exchange and the interoperability of the data. The work is being performed within the frame of the “Emergency Responder Data Interoperability Network (REDIRNET)” project in collaboration with partners such as BAPCO (British Association of Public Safety Officers).

Under the Infrastructure program in research organizations we also provided support services that enable better communications among members of the various research programs, as well as students and their mentors from geographically distributed institutions. The video-conferencing centre provides support for the Simple online com-



Head:  
**Prof. Borka Jerman Blažič**

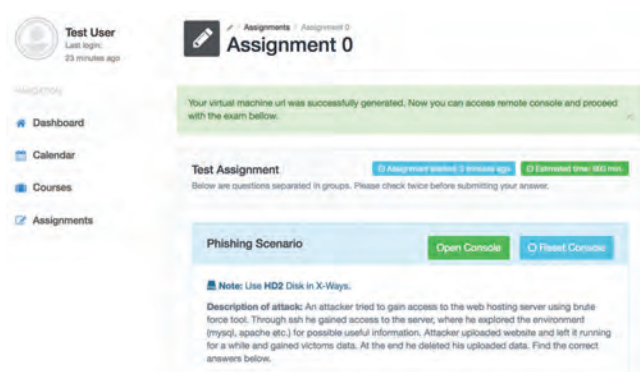


Figure 1: EDUFORS platform

munications and Advanced online communications services, which allow participants a direct view and cooperation at a distance across Europe and around the world, but their use depends on the purpose and complexity of the event.

### **Security, dependability and privacy in information systems**

The provision of security and privacy services is crucial for the modern information society. In 2014 our activities in this field were focused on R&D in security context-aware mechanisms and services for advanced systems and networks, attack modelling on critical infrastructure, privacy issues in mobile networks, and digital forensics.

Context-aware security is a promising approach for overcoming many of the security problems in modern internet networks and systems. Engineering context-aware security solutions for these challenges is difficult, since there is no precise understanding of the notion of the context relevant for security. We have proposed a conceptual model for security context that takes into account related social aspects and defines a set of concepts at the appropriate level of abstraction. The model promises to facilitate the specification, management and reuse of security policies in complex and dynamic environments. A scientific paper with our results was published in the SCI journal "International Journal of Information Security".

In the field of privacy protection in mobile networks and mobile devices, for example, smart phones, we performed an in-depth study of the data-privacy and personal security risks incurred by mobile users in several selected countries, most of them with low scores regarding respect for human rights. First, the technologies available were analysed regarding their capacity to protect the user's privacy and to combat censorship and surveillance. The technical testing provided sufficient information about how security threats can be overcome with additional tools since some smartphone systems do not contain secure technology for personal data protection. Then, the user awareness regarding data protection and privacy was studied. The influence of parameters such as the country's wealth, the state religion and the availability of high technology on user attitudes were explored and discussed. The results have been published in an SCI journal IEEE Technology & Society Magazine.

As part of the "Dynamic Forensics Evaluation and Training (DFET)" project activities from the EU "Prevention of and Fight Against Crime" (ISEC) programme we have created a cloud-based platform for digital forensics education and training, named EDUFORS. The platform enables the automatic and dynamic generation, delivery and evaluation of investigation challenges that law-enforcement officers, students and security specialists have to solve with cyber forensic analytical tools. Currently, three types of scenarios are supported: distributed denial of service, phishing, and SQL injection. An example of the EDUFORS frontend is presented in Figure 1.

Our last international R&D project on information security that started in 2014 is "Cybercrime and cyberterrorism European research agenda (COURAGE)". The main goal of the project is the definition of the R&D agenda in the area of the fight against cybercrime and cyber terrorism. The Laboratory for Open Systems and Networks has the main role in the project in research gap analysis in the field of cybercrime and cyber terrorism.

As part of the research on information security economics we had a scientific monograph published in 2014 with the title "Information security in the business environment: needs, measures and economics of investment". The book presents in detail the latest information security threats and risks, different security services and mechanisms, and methods for optimal investments in the information security technology. The book is beneficial for business companies and students, as well as for security experts. In 2014, we also further developed our structural model, for attack modelling in critical infrastructure, based on attack trees. The model was presented in a book chapter and at several conferences.

### **Technology enhanced learning**

The main goal of the "Scalable cost-effective facilitation of professional identity transformation in public employment services (EmployID)" project that started February 2014 is to support and facilitate the learning process of PES (Public Employment Services) practitioners in their professional identity development. We envision developing a set of services combining and linking eCoaching, reflection, MOOCs, networking, analytical and learning support tools, leading to improved individual and organisational performance in the delivery of employment services. Privacy issues are also being tackled in the project through the development of a concept for handling privacy and ethical aspects on all different levels, ranging from organisational policies, via creating awareness, up to technical measures regarding the ownership and stewardship of data. Our activities also ensure that the tools developed are privacy aware, abide by privacy principles, and are compliant with the newest EU privacy and data-protection legislation. Among the main results of our research activities in 2014 we need to mention the specification of user requirements and contributions to the EmployID conceptual framework and evaluation framework.

### **Science promotion**

For the third time the Laboratory for Open Systems and Networks successfully organized Researchers' Night, with the goal being to promote science, scientists and their results, this year in the frame of the "Meet and Learn

What Excellent Science does for You and the Society (WeForYou) project from the Horizon 2020 programme. The event took place on 26 September 2014 at 12 locations in Ljubljana, Izola, Planica and Novo mesto, where more than 80 lectures, workshops and other events were organized. The main topics of the events were energy, ecology, health and ICT. The Researchers' Night was widely recognized by the broader society, which proved that there is definitely a lack of projects and events with similar contents and that scientists are keen to share their experience with their colleagues and in this way stimulate young people who are just at the beginning of their careers. The estimated total number of visitors at all venues was between 7000 and 8000.

### Some outstanding publications in the past three years

1. Callanan, C., Jerman-Blažič, B.: User understanding of privacy in emerging mobile markets. *IEEE technology & society magazine*, ISSN 0278-0097, 2014, vol. 33, no. 4, 48–56
2. Bojanc, R., Jerman-Blažič, B., Tekavčič, M.: *Informacijska varnost v podjetniškem okolju : potrebe, ukrepi in ekonomika vlaganj*, (Znanstvene monografije Ekonomske fakultete). Ljubljana: Faculty of Economics, 2014. VI, 168 pgs.
3. Jovanovikj, V., Gabrijelčič, D., Klobučar, T.: A conceptual model of security context. *International journal of information security*, ISSN 1615-5262, 2014, vol. 13, no. 6, 571–581

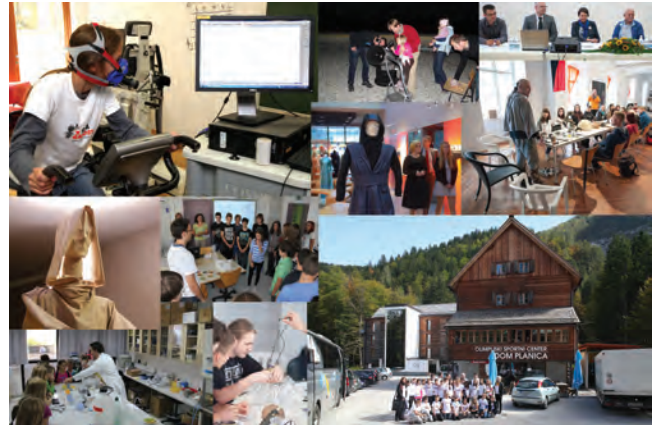


Figure 2: Researchers' Night 2014

### Organization of conferences, congresses and meetings

1. The 2014 Researcher's Night, WEFORYOU - Meet and Learn what excellent science does for you and the society, 26 September 2014
2. Organisation of "EmployID" project meeting, 15–17 October 2014
3. Organization of RedIRNET workshop for first responders, 28 November 2014

## INTERNATIONAL PROJECTS

1. 7FP - COURAGE; Cybercrime and Cyberterrorism (E)uropean Research AGenda  
Prof. Borka Džonova Jerman Blažič  
Slovenian Research Agency
2. 7FP - REDIRNET; Emergency Responder Data Interoperability Network  
Prof. Borka Džonova Jerman Blažič  
European Commission
3. 7FP - EmployID; Scalable Cost-effective Facilitation of Professional Identity Transformation in Public Employment Services  
Asst. Prof. Tomaž Klobučar  
European Commission
4. STORK 2.0; Secure identity across borders Linked 2.0  
Prof. Borka Džonova Jerman Blažič  
European Commission
5. CIP-e-SENS; Electronic Simple European Networked Services  
Prof. Borka Džonova Jerman Blažič  
European Commission
6. D-FET; Dynamic Forensics Evaluation and Training  
Prof. Borka Džonova Jerman Blažič  
European Commission

7. H2020 - WeForYou; Meet and Learn What Excellent Science does for You and the Society  
Asst. Prof. Tanja Arh  
European Commission

## RESEARCH PROGRAM

1. Future Internet Technologies: Concepts, Architectures, Services and Socio-Economic Issues  
Prof. Borka Džonova Jerman Blažič

## R & D GRANTS AND CONTRACTS

1. Content and Data Communication Interoperability of First Responders Networks  
Prof. Borka Džonova Jerman Blažič
2. Future Internet Collaboration Platform  
Prof. Borka Džonova Jerman Blažič
3. Cloud Assisted Services: CC CLASS  
Prof. Borka Džonova Jerman Blažič

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  3. Prof. Borka Džonova Jerman Blažič, Head
  4. Asst. Prof. Tomaž Klobučar
- Postdoctoral associate
5. Dr. Dušan Gabrijelčič
- Postgraduates
6. Blaž Ivanc, B. Sc.
  7. Andrej Jerman Blažič, M. Sc.

8. Maks Mržek, B. Sc., left 13. 03. 14
  9. Tanja Pavleska, B. Sc.
  10. Matija Pipan, M. Sc.
  11. Svetlana Sapelova, left 31. 03. 14
- Technical and administrative staff
12. Primož Cigoj, M. Sc.
  13. Tatjana Martun, B. Sc.

Note:

\* part-time JSI member



# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Cormac Callanan, Borka Jerman-Blažič, "User understanding of privacy in emerging mobile markets", *IEEE technol. soc. mag.*, vol. 33, no. 4, pp. 48-56, 2014.
2. Blaž Ivanc, Tomaž Klobučar, "Attack modeling in the critical infrastructure", *Elektrotehniški vestnik*, vol. 81, no. 5, pp. 285-292, 2014.
3. Vladimir Jovanovikj, Dušan Gabrijelčič, Tomaž Klobučar, "A conceptual model of security context", *Int. j. inf. secur.*, vol. 13, no. 6, pp. 571-581, 2014.
4. Matija Pipan, Julija Lapuh Bele, Dušan Gabrijelčič, "Next generation collaborative platforms in business environments", *Int. j. educ. inf. technol.*, vol. 8, pp. 164-170, 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Borka Jerman-Blažič, "Designing a large cross - border secured eID service for e-government and e-business", In: *ICMS'14, 2014 International Conference on Multimedia Computing and Systems*, April 14-16, 2014, Marrakech, Morocco, [S. l.], IEEE = Institute of Electrical and Electronics Engineers, 2011, 6 pp.
2. Borka Jerman-Blažič, Tanja Arh, Andrej Jerman Blažič, "An approach in the design of virtual environment for e-learning based on usability studies", In: *Proceedings of the 9th International Conference on e-Learning, ICEL-2014, 26-27 June 2014*, Reading, Academic Conferences and Publishing International Limited, 2014, pp. 95-103.
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Blaž Ivanc, "Providing information privacy with attack modeling: from simple techniques to the enhanced structural model", In: *Corporate security: open dilemmas in the modern information society*, Denis Čaleta, ed., Miran Vršec, ed., Blaž Ivanc, ed., Ljubljana, Institute for Corporate Security Studies, 2014, pp. 161-168.

## SCIENTIFIC MONOGRAPH

1. Rok Bojanc, Borka Jerman-Blažič, Metka Tekavčič, *Informacijska varnost v podjetniškem okolju: potrebe, ukrepi in ekonomika vlaganj*, (Znanstvene monografije Ekonomske fakultete), Ljubljana, Ekonomska fakulteta, 2014.

## MENTORING

1. Primož Cigoj, *Cloud computing security and identity management in the OpenStack platform*: master's thesis, Ljubljana, 2014 (mentor Borka Jerman Blažič; co-mentor Tomaž Klobučar).
2. Flamur Abdyli, *How ready are banks in Kosovo to implement an information security policy*: master's thesis, Ljubljana, 2014 (mentor Boštjan Jazbec; co-mentor Borka Jerman Blažič).
3. Marko Beketič, *Economic aspects of information security*: master's thesis, Ljubljana, 2014 (mentor Borka Jerman Blažič).
4. Aleksandra Nerat, *Mobbing in the time of economic and financial crisis*: master's thesis, Maribor, 2014 (mentor Tomaž Klobučar).

# 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 for parallel and distributed computing. Within these activities our research work includes the development of methods and software tools for the modelling, simulation, analysis and synthesis of communication systems, computer simulations supporting biomedical procedures and specialised equipment and procedures for advanced bio-signal processing and interpretation.***

The research and development activities at the department are carried out in the framework of the *Communication Technology Laboratory (CTL)*, the *Parallel and Distributed Systems Laboratory (PDSL)* and the *Networked Embedded Systems Laboratory (NESL)*. The research work of the three laboratories is complementary, which is reflected in the joint applied projects.

In 2014 the research activities within the **Communication Technology Laboratory** were concentrated on different challenges associated with access-segment technologies, enabling end-users to access new multimedia services and applications. As part of the multi-year telecommunication-systems research programme the emphasis was on research in the areas of: radio propagation, access architectures for heterogeneous wireless networks, management of radio and network resources and cognitive communications.

The investigations of radio-signal propagation were 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. 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). We published our research results in the paper "A survey of radio propagation modelling for tunnels", issued in the journal *IEEE Communications Surveys and Tutorials*. The second topic, researched in cooperation with Telekom Slovenije d.d., concerns the development, implementation and testing of software modules for radio-wave propagation modelling in mobile communication systems for rural and urban environments, including statistical channel models as well as channel models based on ray tracing and their integration into the open-source geographic information system (GIS). We have studied computationally efficient radio ray-tracing techniques in the context of graphical pipelines. Building on the new computing possibilities of massively parallel hardware we managed to reduce the excessive running times for many practical applications. Moreover, the optimizations proposed are applicable to a wider set of problems that can be solved on Single Instruction Multiple Data architectures.

We continued the investigation of advanced concepts and technologies for a capacity increase of wireless meshed networks using network-coding techniques. In particular, we focused on the development of advanced network-coding algorithms and their adapted routing procedures. In order to support the performance evaluation of arbitrary network-coding algorithms on predetermined or randomly generated topologies of wireless meshed networks, we designed and built a simulation model that allows the performance evaluation of network-coding algorithms and routing procedures on randomly generated wireless mesh network topologies. We also developed a test bed for the evaluation of a network-coding assisted retransmission scheme for multimedia broadcasting in wireless networks.

In collaboration with European partners within the FP7 ABSOLUTE project (Aerial Base Stations with Opportunistic Links for Unexpected & Temporary Events) we participated in the design and validation of an inno-



Head:  
**Asst. Prof. Mihael Mohorčič**

**We designed and developed new hardware and software modules and implemented new features for the VESNA platform.**

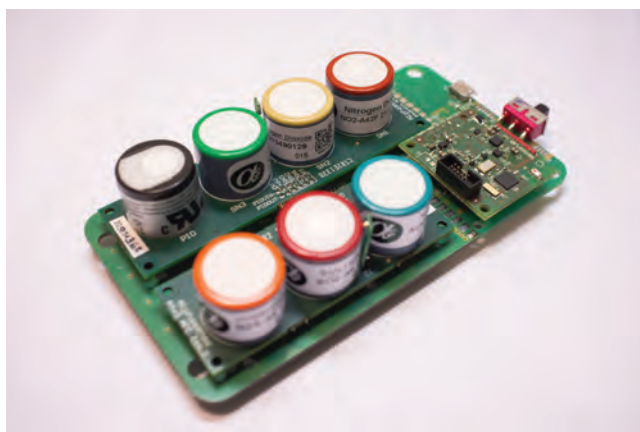


Figure 1: Air-quality monitor based on the VESNA platform.

**In the frame of the EU FP7 CREW project and the FIRE initiative the LOG-a-TEC test bed is used as a real-world outdoor experimental environment for cognitive radio and cognitive networking research.**

**We developed a ground station for receiving satellite signals in the 20- and 40-GHz frequency bands. It is intended for the long-term measurement and modelling of a satellite channel.**

vative, rapidly deployable future network architecture. It should be resilient and capable of providing broadband multi-service, secure and dependable connectivity for large coverage areas affected by large-scale unexpected events (or disasters) leading to the partial or complete unavailability of the terrestrial communication infrastructure, or for temporary events requiring very high throughput and an augmented network capacity. We focused on the development of new, advanced techniques for radio-spectrum manage-

ment, on the development of new network solutions and on the integration of wireless sensor networks into the emergency architecture. We developed a radio-environment map-based simulation model for a capacity assessment of LTE networks.

In 2014 we were actively participating in several COST actions. In the COST Action IC1101 “Optical Wireless Communications – An Emerging Technology” we investigated, in cooperation with TU Graz, the influence of weather conditions on the performance of wireless optical communication systems. We presented and demonstrated the wireless optical system KORUZA, suitable for future gigabit wireless networks. In the COST Action IC1104 “Random Network Coding and Designs over GF(q)”, we are developing practical network coding procedures and evaluating them in a purpose-built simulation model. In the COST action IC1004 “Cooperative Radio Communications for Green Smart Environments” we mainly participate in working groups one and two, with topics related to radio-propagation aspects and problems of the physical layer.

We successfully finished the ESA PECS project SatProSi and started a new SatProSi-Alpha project. In SDR technology we developed a low-cost and high-performance ground station for receiving satellite signals in the 20 and 40 GHz frequency bands. It is intended for the long-term monitoring of the Alphasat carrier and modelling of the satellite channel. We installed one of our own Alphasat receivers at the Hilmwarte site, Graz, Austria, and signed a Memorandum of Understanding with Joanneum Research for the actual exchange, comparison and validation of Alphasat measurement data. In the area of cognitive communications we continued research in the radio and access segments and contributed to the WUN-CogCom and FP7 CREW projects. In 2014 our research in this area was focused on stand-alone and col-

laborative spectrum sensing in licensed and unlicensed frequency bands and on building radio environmental maps. At the beginning of the year, within a new project SUNSEED, we started with research activities in the area of optimization and network management to the field of smart grid networks. In the first year, we focused on the development of modules for the “state estimation” in distribution systems, which are particularly challenging because of their specifics. Our research is interdisciplinary. In cooperation with the Department of Low and Medium Energy Physics we applied the signal-processing techniques known from the field of telecommunications to problems in nuclear spectrometry. In the **Parallel and Distributed Systems Laboratory**, we successfully continued our interdisciplinary research work in the framework of the program group that also includes the Machine Vision Laboratory from the Faculty of Electrical Engineering and the Laboratory for Algorithms and Data Structures from the Faculty of Computer and Information Science, both from the University of Ljubljana. With the two laboratories, we intensively cooperated on two running research projects. We also cooperate with researchers from industry (the former Turboinstitut d.d. and Xlab d.o.o.) and from the medical sphere (the University Medical Centre Ljubljana).

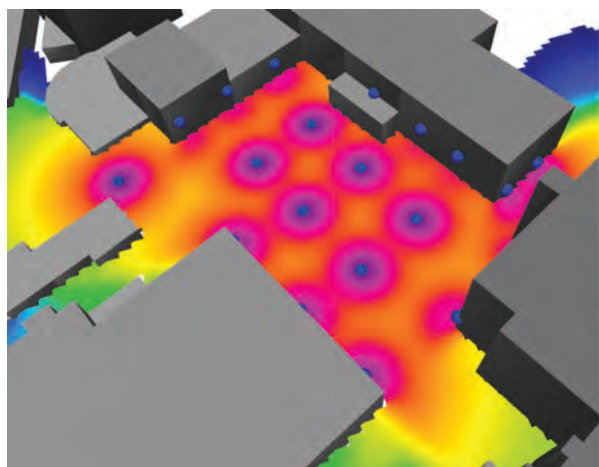


Figure 2: Sensor-node locations and radio coverage of experimental sensor network test bed at the Jožef Stefan Institute.

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**We proposed a new data-flow-based method for the data-flow parallelization of the search in searching for n-connected components.**

We investigated computer algorithms efficiently implementable on parallel and distributed computers. We tested them on a 152-core computer cluster stationed in our department and reachable also within a cloud, which we have established in cooperation with our research and industrial partners. Besides demanding computations, we paid attention to the distributed storage of large amounts of data. We continued investigations in the field of

wireless sensor networks based on the theory of parallel and distributed computing and communication.

**We demonstrated that in the numerical simulation of natural phenomena, a local meshless approach can result in a superlinear speedup when using a local meshless approach in the numerical simulation of natural phenomena.**

On the initiative of an industrial partner, we developed a strategy for the modelling and simulation of the icing on overhead electrical lines and for an experimental evaluation of the obtained results. The final goal is the operative forecasting and prevention of the icing on high-voltage overhead



lines. Our partners in the project are Elektoinstitut Milan Vidmar and the Slovenian Environment Agency.

We tested the efficiency of new, parallel, numerical algorithms that can be executed on parallel computers, e.g., the efficiency of local meshless methods. With these methods, we simulated various physical phenomena (e.g., heat, mass and momentum transport and multi-phase flows) and semiconductors in realistic circumstances. For a better understanding of the optimization based on simulations performed in a parallel and distributed environment, we employed methods of multi-criteria optimization.

These investigations are expected to enable even tighter coupling between the optimization and simulations, and thereby highly efficient simulations of physical phenomena.

In the area of thermal therapy, we acquired a Slovenian patent and applied for an international one for a method and a device with which, during therapeutic cooling or heating, one can in real time and in line with the desired protocol non-invasively control inner body temperature variables that are difficult or impossible to measure directly. The method and the device use computer simulations, machine learning and system control techniques.

We further developed our new methodology for synthesising the standard ECG from a small number of differential measurements. Methods for extracting the breathing signal from ECG recordings have been developed. Together with neurologists from the University Medical Centre Ljubljana, we continue with equipment upgrading and measurements for the in-house developed program environment NeuroECG.

We further developed and produced the first batch of fully functional wearable ECG measuring-device prototypes. The usage of such devices was enabled by the recent advances in wireless data-transfer technologies, namely, of the Bluetooth Smart technology and of smart phones and tablets that fully support it. The ECG measuring device is small, unobtrusive when worn, transmits the measurements wirelessly and is able to work on battery power for a few days. Devices like this one will represent the base of future telemedicine and telehealth services, which are indispensable for lowering the costs of the general health services.

In the area of computer-supported biomedical research, after a successful presentation of spontaneous cardio-inhibitory syncope, we continued the research of the impact of myocardial revascularization on the fractal heartbeat dynamics. The latter is also related to the atrial activity (P waves) and to the complex structures of the sinus node and its functional pacemaker areas, where the atrial activity strongly depends on the influences of the autonomic nervous system on the sinoatrial node. For signal processing, we employed advanced computer algorithms that in the case of large amounts of data need to be executed on parallel computers. In collaboration with researchers and physicians from the University Medical Centre Ljubljana and the University Clinic of Pulmonary and Allergic Diseases Golnik, we completed a research study of heart-rate variability in patients with chronic obstructive pulmonary disease in rehabilitation conditions, and published our first results in an eminent international journal.

In the field of formal methods for discrete systems development, we investigated the synthesis of complete test suites for final state machines and proposed numerous generalizations and improvements to the existing algorithms. In cooperation with the University of Podgorica, we developed and published a new algorithm for the analysis of n-connectivity in 2D cell arrays, which can be efficiently implemented with cellular automata.

In 2014 the Networked Embedded Systems Laboratory mainly focused on research and development in the areas of the Internet of Things and cognitive communications. The emphasis was on the vertical integration of different wireless sensor and communication network technologies with

**We explained to some extent the impact of myocardial revascularization on the fractal heartbeat dynamics of heart beating and presented the results of a clinical study about heart-rate variability in patients with chronic obstructive pulmonary disease in the rehabilitation process conditions.**

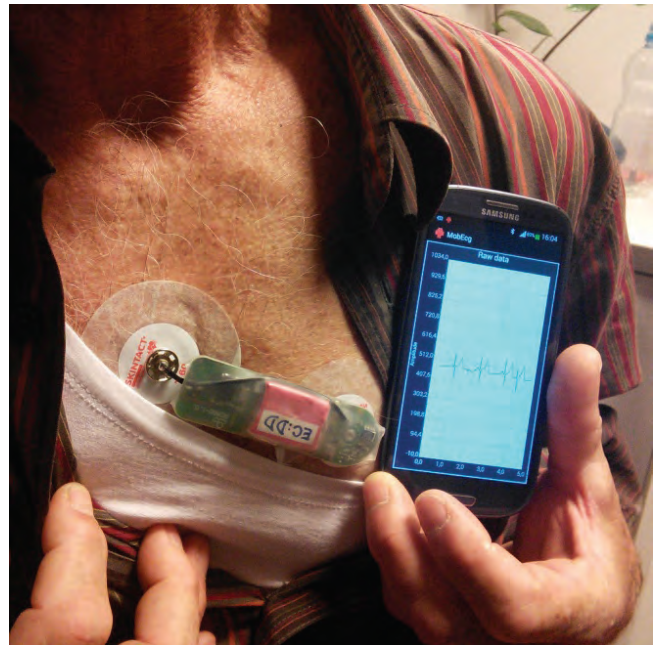


Figure 3: Prototype model of a miniature multifunctional body sensor that measures ECG, movements, temperature, light, and moisture, thereby associating physiological measurements with the context of the environment.

**We developed a new methodology for the simulation of semiconductors and evaluated it on the test case of a PN junction.**

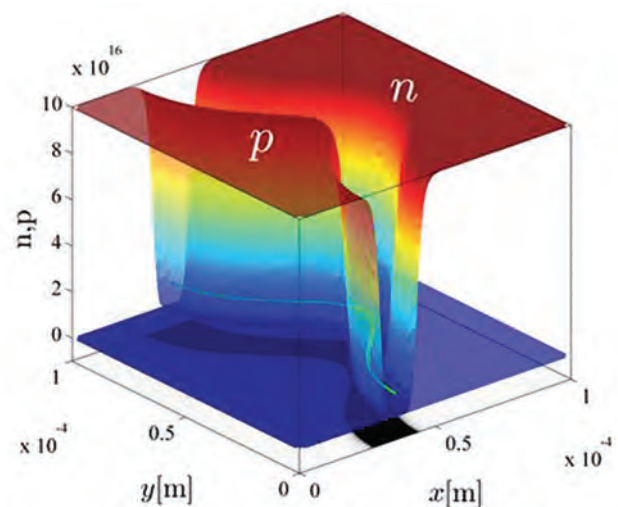


Figure 4: Distribution of holes and electrons within a non-uniform PN junction as calculated with a parallel implementation of a meshless numerical method for the simulation of semiconductors.



semantic technologies in support of the autonomous search and composition of sensors and sensor data, as well as on the development of new applications using various machine-learning and decision-making algorithms. These activities were mainly conducted within the basic research program “Telecommunication systems” and the EU FP7 Network of Excellence PlanetData.

The modular and fully flexible platform VESNA for wireless sensor networks and existing external modules, developed as the core building blocks for several research and applied projects, was completely redesigned and upgraded with a set of new features. A set of new models was also designed and implemented. New software based

**We signed a Memorandum of Understanding with Joanneum Research for the exchange, comparison and validation of Alphasat measurement data.**

on the Contiki OS was developed. The redesign and implementation of a new radio-spectrum sensing module in the UHF and VHF frequency bands was finished. The development of ProtoStack, a tool for remote composition, reconfiguration and reprogramming of the CRime protocol stack, is continuing. A variety of supported features, protocols and technologies, together with an arbitrary combination of developed hardware and software modules, make

the VESNA platform well suited to the implementation of an experimental research sensor networks infrastructure, the deployment of pilot applications, the validation of usage scenarios and the development of end-user solutions.

A new test bed at the premises of the Jožef Stefan Institute has been setup for the needs of experiments in a real urban environment. The large-scale outdoor wireless sensor network LOG-a-TEC experimental test bed, setup in collaboration with the Municipality of Logatec and Komunalno podjetje Logatec, was upgraded. The remote sensor nodes' firmware management, the remote execution of experiments and the remote gathering of sensor measurements data via a web application running on one of our servers is also upgraded. The experimental test bed located in Logatec was applied for a comparison of the measured and predicted DVB-T signal within the CREW project. The new module for spectrum sensing in the UHF and VHF frequency bands was employed in an experiment for spectrum sensing in London, which was performed in cooperation with OFCOM, the UK spectrum regulator. Several experiments were performed in Logatec within the Crew project, mainly related to the spectrum assignment of unlicensed spectrum and the use of geolocation databases.

In the area of wireless sensor networks we continued two FP7 projects, namely, ABSOLUTE and CITI-SENSE. In the ABSOLUTE project our role is to integrate the VESNA-based wireless sensor network in the emergency communications network architecture. The aim is to provide aneasily deployable sensor network for in-situ fixed or participatory monitoring of post-disaster parameters as well as for the spectrum sensing needed to support the

ad-hoc establishment of the ABSOLUTE communication system without causing harmful interference to coexisting communication systems. In this respect, we designed, implemented and integrated the sensor network into a portable land mobile unit, which in addition to sensing the environmental parameters, includes a GPS module and a unit for the control of power consumption in a portable land mobile unit. In the CITI-SENSE project, which is concerned with the establishment of sensor-based Citizens' Observatory Community for improving the quality of life in cities, our focus was mainly on providing the VESNA-based solution for air-quality monitoring. As part of this we developed the module with gas, particle matter and other ambient related sensors, which by using Wi-Fi connectivity sends measured data to smart phone or tablet. The role of the smart phone is twofold. It is applied for graphical presentation of measured data and as a relay for sending data to a remote data server.

In 2014, we continued with two technology development projects financed by the Ministry of Economic Development and Technology SMER+, namely, “Smart camper” and “Smart home”. In the first one, we are developing sensor and communication technologies for the intelligent remote management of motorhomes. Within the project we developed a VESNA-based controller. Six of them were integrated into the next-generation motorhome designed and produced by the company Adria Mobil. The integrated modules are connected to a central processing unit, the role of which is in data collection and processing. Based on measured data, intelligent algorithms found out the habits of motorhome users and predict the use of motorhome resources. The system also supports connection to a smart phone and central data collection. In the second project, together with the company Cosylab, we are developing sensor and communication technologies for smart buildings, with an emphasis on monitoring the generation and consumption of electricity.

Within the FP7 project SUNSEED and in collaboration with Elektro Primorska, the Networked Embedded Systems Laboratory started the development of a sensor platform for measuring electricity consumption, current, voltage, frequency and distortion factor at the electricity consumers in this year. The platform will be shown at the “Mobile World Congress 2015” in Barcelona.



Figure 5: Design load of GRID network at the Kromberk test bed

In the collaboration with the company Hella within the project ProaSense, the aim of which is to design an innovative and comprehensive approach to proactive intelligence, information management, problem solving and decision support, we are predicting the quality of headlights from measured environmental and production parameters.

At the end of this year we started a new project "Observe, Reason, Act (OSU)" supported by Ministry of Education, Science and Sport. The main aim of the project is to develop a learning tool that enables the remote collection, reviewing and analysis of data, as well as the simple adding of additional data sources.

The Networked Embedded Systems Laboratory and its research and development activities also take part in the SensorLab group, which was established by the Department of Communication Systems and the Laboratory of Artificial Intelligence.

## Some outstanding publications in the past year

1. Hrovat, A., Kandus, G., Javornik, T.: A survey of radio propagation modeling for tunnels. *IEEE Communications surveys and tutorials*, 2014, vol. 16, no. 2, 658–669, doi: 10.1109/SURV.2013.091213.00175
2. Novak, R.: Loop optimization for divergence reduction on GPUs with SIMT architecture. *IEEE transactions on parallel and distributed systems*, [in press] 2014, 10 pgs., doi: 10.1109/TPDS.2014.2324587
3. Fortuna, C., Mohorčič, M.: A framework for dynamic composition of communication services. *ACM transactions on sensor networks*, [in press] 2014, 10 pgs., doi: 10.1145/2678216
4. Tomašič, I., Trobec, R.: Electrocardiographic systems with reduced numbers of leads - synthesis of the 12-lead ECG. *IEEE reviews in biomedical engineering*, 2014, vol. 7, 126–142, doi: 10.1109/RBME.2013.2264282
5. Kšela, J., Avbelj, V., Kališnik, J.-M.: The impact of beating-heart myocardial revascularization on multifractal properties of heartbeat dynamics. *International journal of cardiology*, 2014, vol. 177, no. 3, 1111–1112, doi: 10.1016/j.ijcard.2014.08.083
6. Županič, E., Živanovič, I., Kališnik, J.-M., Avbelj, V., Lainščak, M.: The effect of 4-week rehabilitation on heart rate variability and QTc interval in patients with chronic obstructive pulmonary disease. *COPD*, ISSN 1541-2555, 2014, vol. 11, no. 6, 659–669, doi: 10.3109/15412555.2014.898046
7. Rashkovska, A., Trobec, R., Avbelj, V., Veselko, M.: Knee temperatures measured in vivo after arthroscopic ACL reconstruction followed by cryotherapy with gel-packs or computer controlled heat extraction. *Knee surgery, sports traumatology, arthroscopy*, ISSN 0942-2056, 2014, vol. 22, no. 9, 2048–2056, doi: 10.1007/s00167-013-2605-x
8. Kosec, G., Depolli, M., Rashkovska, A., Trobec, R.: Super linear speedup in a local parallel meshless solution of thermo-fluid problem. *Computers & Structures*, ISSN 0045-7949. [Print ed.], 2014, vol. 133, 30–38, doi: 10.1016/j.compstruc.2013.11.016

## Awards and appointments

1. Hekovnik Prize for "Mobilni EKG" in the frame of the programme start:Something, 21 November 2014
2. Dr. Gregor Kosec: Emerald's awards for excellence: Engineering Outstanding Doctoral Research, Emerald's awards for excellence: Outstanding paper. Second International Conference on Computational Methods for Thermal Problems (ThermaComp 2011), Dalian, China, Solution of a low Prandtl number natural convection benchmark by a local meshless method. V. LI, X. (ur.), 5-7 September 2011, (International Journal of Numerical Methods for Heat & Fluid Flow, ISSN 0961-5539, vol. 23, no. 1). Bradford: Emerald, 2013, vol. 23, no. 1, 189-204

## Organization of conferences, congresses and meetings

1. CREW annual review meeting, Ljubljana, Slovenia 19-22 November 2014
2. International Conference "DC VIS / Distributed Computing, Visualization and Biomedical Engineering" in the frame of the international convention MIPRO 2014, Opatija, Croatia, 26-30 May 2014
3. Workshop HiPEAC (European Network of Excellence on high Performance and Embedded Architecture and Compilation), Ljubljana, 25 September 2014

## Patents granted

1. Aleksandra Rashkovska, Roman Trobec, A procedure and a device for non-invasive control of internal temperature variables in real time between therapy with cooling and heating, SI24357 (A), Urad RS za intelektualno lastnino, 28.11.2014.

- Roman Trobec, Procedure and device for word context window deployment, SI24263 (A), Urad RS za intelektualno lastnino, 30.6.2014.

## INTERNATIONAL PROJECTS

- 7FP - PlanetData  
Asst. Prof. Mihael Mohorčič  
European Commission
- 7FP - CREW; Cognitive Radio Experimentation World  
Asst. Prof. Mihael Mohorčič  
European Commission
- 7FP - ABSOLUTE; Aerial Base Stations with Opportunistic Links for Unexpected and Temporary Events  
Asst. Prof. Mihael Mohorčič  
European Commission
- 7FP - CITI-SENSE; Development of Sensor-based Citizens' Observatory Community for Improving Quality of Life in Cities  
Asst. Prof. Mihael Mohorčič  
European Commission
- 7FP - VHP NoE; Virtual Physiological Human Network of Excellence  
Prof. Roman Trobec  
European Commission
- 7FP - ProaSense; The Proactive Sensing Enterprise  
Asst. Prof. Mihael Mohorčič  
European Commission
- 7FP - SUNSEED; Sustainable and Robust Networking for Smart Electricity Distribution  
Asst. Prof. Mihael Mohorčič  
European Commission
- 7FP - Fed4FIRE; Federation for FIRE - Federation for Future Internet Research and Experimentation  
Asst. Prof. Mihael Mohorčič  
European Commission
- ESA PECS; Processing of Satellite Signals in Ka/Q-frequency Band  
Prof. Gorazd Kandus  
ESA/ESTEC.
- ESA - SatProSi-Alpha; Ka/Q-band Propagation Measurements and Modelling - Slovenian Contribution to the Alphasat TDP#5 Scientific Mission  
Dr. Andrej Vilhar  
ESA/ESTEC.
- COST IC1004; Cooperative Radio Communications for Green Smart Environments  
Asst. Prof. Tomaž Javornik  
COST Office
- COST IC1101; Optical Wireless Communications - An Emerging Technology  
Prof. Gorazd Kandus  
COST Office
- COST IC0906; WiNeMO; Wireless Networking for Moving Objects  
Miha Smolnikar, B. Sc.  
COST Office

- COST IC1104; Random Network Coding and Designs over GF(q)  
Asst. Prof. Aleš Švigelj

## RESEARCH PROGRAMS

- Telecommunication Systems  
Prof. Gorazd Kandus
- Parallel and Distributed Systems  
Prof. Roman Trobec

## R & D GRANTS AND CONTRACTS

- 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
- Model for Domain-Specific Trend Prediction based on Semantic Enrichment of Unstructured Patterns  
Prof. Roman Trobec
- Open Communication Platform for Service Integration: CC OPCOMM  
Asst. Prof. Mihael Mohorčič
- Cloud Assisted Services: CC CLASS  
Prof. Roman Trobec
- Efficient Self-Configuration Methods for Wireless Mesh Networks  
Dr. Carolina Fortuna
- Observe, Infer, Act  
Asst. Prof. Mihael Mohorčič
- HiPEAC; European Network of Excellence on High Performance and Embedded Architecture and Compilation  
Prof. Roman Trobec

## NEW CONTRACTS

- Technologies for Next-Generation Intelligent Motorhome  
Asst. Prof. Mihael Mohorčič  
Adria Mobil, d. o. o., Novo mesto
- Propagation and Topology Design Evaluation for Wireless Sensor Networks Operating in License Exempt Frequency Bands  
Asst. Prof. Mihael Mohorčič  
Cosylab, laboratorij za kontrolne sisteme, d. d.

## VISITOR FROM ABROAD

- Dr. Mihai Suci, Technical University of Cluj-Napoca, Faculty for Electronics, Telecommunications and Information Technology, Cluj-Napoca, Romania, 10 March-9 June 2014

## STAFF

### Researchers

- Dr. Viktor Avbelj
- Dr. Andrej Hrovat
- Asst. Prof. Tomaž Javornik
- Prof. Gorazd Kandus
- Prof. Monika Kapus Kolar
- Asst. Prof. Andrej Lipej\*
- Asst. Prof. Mihael Mohorčič, Head
- Asst. Prof. Roman Novak
- Dr. Igor Ozimek
- Dr. Marjan Šterk\*, left 01. 03. 14
- Asst. Prof. Aleš Švigelj
- Prof. Roman Trobec

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- Dr. Carolina Fortuna
- Dr. Gregor Kosec
- Dr. Aleksandra Rashkovska

- Dr. Andrej Vilhar

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  - Jernej Hribar, B. Sc.
  - Urban Kuhar, B. Sc.
  - Erik Pertout, B. Sc., left 01. 07. 14
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  - Matevž Vučnik, B. Sc.
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  - Tomaž Krištofelc
  - Miha Smolnikar, B. Sc.
  - Polonca Šega, B. Sc.

Note:

\* part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

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- Ciprian Anton, Andrei Toma, Ligia Cremene, Mihael Mohorčič, Carolina Fortuna, "Power allocation game for interference mitigation in a real-world experimental testbed", In: *Proceedings*, IEEE International Conference on Communications, ICC 2014, and Sydney, Australia gedited by Abbas Jamalipour and Der-Jiunn Deng, Abbas Jamalipour, ed., Der-Jiunn Deng, ed., Denver, IEEE, 2014, pp. 1501-1507.
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  15. Carlo Riva et al. (11 authors), "The Aldo Paraboni scientific experiment: the European measurement campaign", In: *Moving forward: 2014 conference*, (Proceedings, vol. 2/3), [S. l., s. n.], 2014, pp. 367-375.
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  17. Radovan Zentner, Andrej Hrovat, Nikola Mataga, "Derivation and application of ray entity concept", In: *URSI GAS 2014*, 31st General Assembly of the International Union of Radio Science, August 16-23, 2014, Beijing, China, [S. l., s. n.], 2014, 4 pp.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Matjaž Depolli, Gregor Kosec, Roman Trobec, "Efficient numerical solution of 2D diffusion equation on multicore computers", In: *High-performance computing on complex environments*, Emmanuel Jeannot, ed., Julius Zilinskas, ed., new York, Wiley, 2014, pp. 33-51.

## PATENT

1. Aleksandra Rashkovska, Roman Trobec, *A procedure and a device for non-invasive control of internal temperature variables in real time between therapy with cooling and heating*, SI24357 (A), Urad RS za intelektualno lastnino, 28.11.2014.
2. Roman Trobec, *Procedure and device for word context window deployment*, SI24263 (A), Urad RS za intelektualno lastnino, 30.6.2014.

## MENTORING

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# COMPUTER SYSTEMS DEPARTMENT

## E-7

*The Computer Systems Department is concerned primarily with the development of advanced computing structures and efficient algorithms for massive-data processing, and systems for effective human-computer interaction. Within this broad area, we are concentrating on self-reparable and self-organizing systems, the modelling and optimizing of complex, dynamic and nondeterministic systems. Our research results are implemented within applications for production, transport, energy, environmental sustainability, bioinformatics, health, and medicine. As an integral part of our research activities, members of the department have close contacts and collaborations with scientists around the world, through academic links and industrial contacts, thus enabling us to keep at the forefront of rapidly developing fields.*

### Advanced computer structures for data processing

In the field of advanced computer structures we continued the development of self-reparable systems based on FPGA. The SRAM-based field-programmable gate arrays (FPGAs) in mission-critical systems require error-mitigation and recovery techniques to protect them from the errors caused by high-energy radiation, also known as single-event upsets (SEUs). The developed SEU-recovery mechanism has a smaller hardware overhead than the existing solutions. According to the required levels of reliability, different architectures of the self-recoverable mechanism can be employed. The results of our work on the error-recovery mechanism in FPGA using a dynamic partial reconfiguration were presented at the TRUDEVICE Workshop on Test and Fault Tolerance for Secure Devices conducted in the frame of COST action IC1204.

Dynamic partial reconfiguration was used to implement the PCI Express interface on FPGA device. Full configuration of the FPGA design cannot be completed during the PCI-E enumeration process defined by the PCI Express specification. The developed PCI-E interface is split into two parts. The static part is as small as possible to achieve enumeration timing, containing only the essential parts of the PCI Express interface. The reconfigurable part that contains most of the user design is performed after the system PCI-E enumeration. The developed PCI-E interface can be reused in the design of various FPGA accelerated systems.

We developed electronic circuits with advanced functionalities. In collaboration with BSH Hišni aparati, d.o.o., Nazarje, we upgraded the electronic circuits in their MaxxiMUM series of household appliances. We implemented several additional functionalities, and improved their usability. The developed a microcontroller and additional sensors, as well as an application for tablet mobile devices, allow the remote monitoring and control of the appliances, while still allowing unchanged functionalities of the original appliances, where the functionality of the SensorControl is fully employed.

We addressed the issue of the measurement accuracy of an oscillation-based test of a generic Fleischer-Laker biquad switched-capacitor (SC) filter stage. The theoretical framework for the analysis of the impact of the non-ideal characteristics of the circuit components on the resulting oscillation frequency has been developed. The efficiency of the proposed oscillation-based test schemes of SC biquad filters has been verified in terms of the achieved fault coverage and a comparison with other test methods has been performed on a selected case study.

### Efficient algorithms for computer data processing

Research in the field of developing efficient algorithms for computer data processing was focused on the development of computer support for diet planning.

In the FP7 European project Quantify Life - Feed Yourself - QuaLiFY (<http://qualify-fp7.eu>) we lead the workpackage on the development of the QuaLiFY server platform, where data and services will be available for individual nutritional treatments and recommendations. The stress is on the scientific proof of quality of data and services. Our contribution to the platform will be the service for menu planning, considering several constraints and criteria.



Head (since 9. 12. 2014):

**Asst. Prof. Gregor Papa**



Head (until 8. 12. 2014):

**Prof. Franc Novak**

**Dynamic partial reconfiguration was implemented in secure devices.**

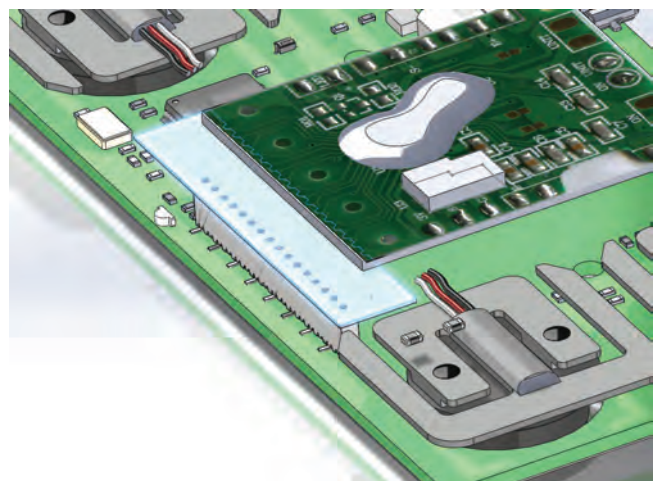


Figure 1: The circuit of the portable kitchen-scales

Within the FP7 European ERA Chair ISO-FOOD (<http://isofood.eu>), in the field of isotope stability with the aim of ensuring food quality, safety and traceability, we lead the horizontal area of knowledge repository. We develop databases and a knowledge base in the area of foodomics, tools for data handling, and methods for the extraction, management and analysis of data and knowledge.

In the **Libra** project (<http://nutri.si>) for the Ministry of Health we developed a portable kitchen scale with the size of a smart-phone that allows simple food weighing. The scale is connected through a wireless Bluetooth connection to a mobile application Nutri, which allows carbohydrate counting in the weighed food. Since the application is also wirelessly connected to a glucose meter it allows the calculation of bolus insulin doses to correct user's meal-time glucose level. The Libra scale was developed with the use

**Development of simulation framework to support planning and optimization of city-traffic flows.**

of a simple acquisition and transfer method. The Nutri application is connected with the web application OPEN (Open platform for clinical nutrition, <http://opkp.si>), which is also the result of our development. The preliminary results of the clinical study among the diabetes patients, performed at the General Hospital Novo mesto, proved the simplicity of using both the scale and the application.

In cooperation with the National Institute of Public Health, Regional Unit of Kranj, we developed, within the web portal **Šolski lonec** (<http://solskilonec.si>), a web tool for menu planning. This tool allows a connection with the OPKP web application and is implemented as a plug-in for the Wordpress web software for website creation.

In the field of **self-organizing systems** we worked on the parameter-less and **self-adaptive control** of the optimization algorithms. The effectiveness of the approach, where the user does not need any specific knowledge of the control-parameter setting, was tested in the context of multi-criteria optimization. An additional usability of the approach is seen in connection with self-organizing emergent systems. For this reason, we study stigmergy, i.e., coordination, where the collective functioning of the system is achieved by indirect interactions between the elements of the system. We investigate both sematectonic and sign-based stigmergy. Sematectonic stigmergy denotes communication via the modification of a physical environment, while sign-based stigmergy denotes communication via a signalling mechanism.

The principle of self-organizing stigmergic systems is used in the implementation of the solutions for optimization procedures within the ARTEMIS project **Adaptive Cooperative Control in Urban (sub) Systems - ACCUS** (<http://www.projectaccus.eu/>), where we are developing the platform for the integration and coordination of urban systems (transportation, outdoor lighting, energy) to build applications across urban systems, to provide adaptive and cooperative control for urban subsystems, and to optimize their combined performance.

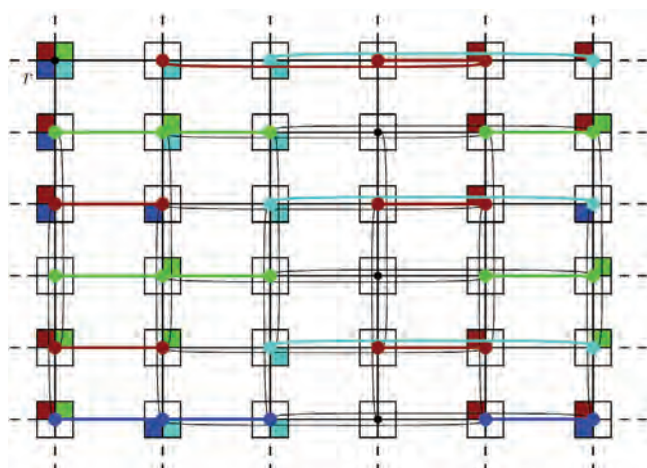
The theoretical research on **simultaneous information transfer through a network** was carried out. We are interested in the problem of transferring different information from a given unit (node) through a network, where

each node is able to transfer only one packet of information at a time. To achieve a smooth information transfer we restrict it so that each node can process only one packet of information at a time. We examine efficient ways of information transfer, such that all messages reach all parts of the network, i.e., efficient broadcasting. Primarily, we are interested in networks that can be represented as Cartesian products, for which we found an efficient scheme of broadcasting. We presented a family of networks, where under the given conditions, the proposed scheme gives us a solution that is optimal with respect to time.

We are developing a **traffic-flow simulation** framework, based on the OpenDRIVE logical description of a road network. The framework includes descriptions of the road network and traffic lights and allows the simulation of vehicle flows, according to the IDM (Intelligent driver model). Basically, the simulator allows the planning of new and/or changed road segments, since their influence can be easily observed. The simulator is upgraded to allow the optimization of the traffic flow, with the aim being to optimize the traffic lights' switch segments, resulting in more fluent traffic flows.

In cooperation with the Department of Intelligent Systems we organized one of the most important conferences, with a wide response in the

field of natural computing, the 13th International Conference on **Parallel Problem Solving from Nature (PPSN XIII)**. The conference took place during the period September 13-17 in Ljubljana. This biennial scientific conference brings together researchers and practitioners from the field of natural computing. In addition to keynote and regular presentations, the conference featured workshops and tutorials covering advanced topics in this field. The conference was attended by 180 participants from 28 countries around the world.



*Figure 2: Simultaneous information transfer through the network, where large-size information is transferred through the network in smaller packets, which are denoted by different colours.*

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 eleventh consecutive year, the workshops on **Nature-inspired algorithms** about stochastic optimization techniques.

#### Human-computer interaction

In the area of human-computer interaction we continued with the development of a **website usability testing tool**, which was initially designed in collaboration with the Faculty of Electrical Engineering and Computer Science, University of Maribor. We started with the design of software tools for the eyetracker unit.

In cooperation of the Faculty of Computer and Information Science, University of Ljubljana, XLAB Research, Ljubljana, and the Jožef Stefan Institute that form the core partners of the informal community **Slovenian human-computer interaction researchers** (<http://hci.si/>), we organized the conference Human-computer Interaction in Information Society, in the frame of the 17th international Information Society multiconference.

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 electroporation treatment. A new version of the software application was implemented, which helps researchers to quickly obtain the number of biological cells in a large number of image series by manually counting cells in only a few images. The tested accuracy is over 90%, which is comparable to user manual counting; especially taking into account inter-person error, which can be up to 10%.

In collaboration with the Faculty of Health Studies, University of Ljubljana, we continued the work on the **Wartenberg pendulum** test where a time dependence of the knee angle is tracked and then compared to a damped oscillation curve. The parameters of this curve are used to determine the viscosity of a knee's synovial fluid and to detect anomalies. Several groups of people were tested, belonging to different age populations, some of them being affected by diabetes.

In the area of **pattern recognition** we started new research in the field of **automatic classification of heart diseases** using auscultation signals from a digital stethoscope. The first result is a method for the automatic classification of pathologic and physiologic heart murmur with high accuracy. The procedure is based on a machine-learning classification of power spectra within systolic and diastolic period.

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**Co-organization of an important international conference on Parallel Problem Solving from Nature (PPSN XIII).**

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### Some outstanding publications in the past year

1. Vukašinović, V., Šilc, J., Škrekovski, R.: Modeling acquaintance networks based on balance theory, *International journal of applied mathematics and computer science*, 24 (2014) 3, 683-696
2. Benedičič, L., Cruz, F. A., Hamada, T., Korošec, P.: A GRASS GIS parallel module for radio-propagation prediction", *International journal of geographical information science*, 28 (2014) 4, 799-823
3. Bole, U., Popovič, A., Žabkar, J., Papa, G., Jaklič, J.: A case analysis of embryonic data mining success, *International journal of information management*, [in press] (2014), 7
4. Kač, U., Novak, F.: Practical considerations in oscillation based test of SC biquad filters, *Information technology and control*, 43 (2014) 1, 28-36
5. Benedik, E., Koroušič Seljak, B., Simčič, M., Rogelj, I., Bratanič, B., Ding, E. L., Orel, R., Fidler Mis, N.: Comparison of paper- and web-based dietary records: a pilot study, *Annals of nutrition and metabolism*, 64 (2014) 2, 156-166

### Organization of Conferences, Congresses and Meetings

1. AVN, The 24th Workshop Nature-Inspired Algorithms, Ljubljana, Slovenia, 23. 5. 2014
2. HCI-IS 2014, Human-Computer Interaction in Information Society, 17th international Information Society - IS 2014 multiconference, Ljubljana, Slovenia, 8. 10. 2014
3. BIOMA 2014, Student workshop on Bioinspired Optimization Methods and their Applications, Ljubljana, Slovenia, 13. 9. 2014
4. PPSN 2014, 13th International Conference on Parallel problem Solving from Nature, Ljubljana, Slovenia, 13.-17. 9. 2014
5. AVN, The 25th Workshop Nature-Inspired Algorithms, Maribor, Slovenia, 10. 12. 2014



## INTERNATIONAL PROJECTS

1. 7FP - QuaLiFY; Quantify Life - Feed Yourself  
Asst. Prof. Barbara Koroušič Seljak  
European Commission
2. 7 FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability  
Asst. Prof. Barbara Koroušič Seljak  
European Commission
3. COST IC1204; Trustworthy Manufacturing and Utilization of Secure Devices  
Prof. Franc Novak  
COST Office
3. Upgrade of the Open Platform for Clinical Nutrition to Suit the Needs of the Federation of EU Member National Associations of Dietitians EFAD  
Asst. Prof. Barbara Koroušič Seljak
4. Adaptive Cooperative Control in Urban (sub) Systems  
Asst. Prof. Gregor Papa
5. Diabetes Tracker Mobile Application and Pocket-Size Scale (LIBRA)  
Asst. Prof. Barbara Koroušič Seljak
6. Establishment of a Comprehensive System of e-Support Implementation of the Guidelines for Healthy Meals in Educational Institutions in the Republic of Slovenia-The e-School Meals Professional Support - ESMS (In Slovene - ESPO)  
Asst. Prof. Barbara Koroušič Seljak
7. EuroDISH; EuroDISH Determinants-Intake-Status-Health  
Asst. Prof. Barbara Koroušič Seljak

## RESEARCH PROGRAM

1. Computer Structures and Systems  
Prof. Stanislav Kováčič

## R & D GRANTS AND CONTRACTS

1. HiPEAC; European Network of Excellence on High Performance and Embedded Architecture and Compilation  
Prof. Franc Novak
2. EuroFIR AISBL Infrastructure Consultancy  
Prof. Peter Korošec

## NEW CONTRACTS

1. Analysis of Possible Upgrades of the A-Portal Web Platform  
Asst. Prof. Gregor Papa  
Abak.net, d. o. o.
2. Study of the Effects of Upgrading on ISL Online Software  
Asst. Prof. Gregor Papa  
Xlab, d. o. o.
3. The Development of WiFi Direct Prototype  
Asst. Prof. Gregor Papa  
BSH Home Appliances Group

## VISITORS FROM ABROAD

1. Prof. Marian Vajteršič, Institute of Computer Sciences, University of Salzburg, Salzburg, Austria and Institute of Mathematics, Slovak Academy of Sciences, Bratislava, Slovakia, 25.-27. 2. 2014
2. Jim Cooling, Lindentree Associates, Markfield, United Kingdom, 24.-30. 6. 2014
3. Prof. Paul Finglas, Institute of Food Research, Norwich, United Kingdom, 29.-30. 10. 2014
4. Prof. Petr Gregor, Charles University in Prague, Faculty of Mathematics and Physics, Prague, Czech Republic, 11.-18. 11. 2014

## STAFF

### Researchers

1. Asst. Prof. Anton Biasizzo
2. Prof. Peter Korošec
3. Asst. Prof. Barbara Koroušič Seljak
4. Prof. Stanislav Kováčič\*
5. Prof. Franc Novak
6. Asst. Prof. Gregor Papa, Head
7. Asst. Prof. Jurij Šilc

### Postdoctoral associates

8. Dr. Drago Torkar

9. Dr. Vida Vukašinović  
**Technical officer**
10. Marko Pavlin\*, M. Sc.  
**Technical and administrative staff**
11. Jolanda Jakofčič

### Note:

\* part-time JSI member

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Lucas Benedičič, Felipe A. Cruz, Tsuyoshi Hamada, Peter Korošec, "A GRASS GIS parallel module for radio-propagation predictions", *International journal of geographical information science*, vol. 28, issue 4, pp. 799-823, 2014.
2. Lucas Benedičič, Marko Pesko, Tomaž Javornik, Peter Korošec, "A metaheuristic approach for propagation-model tuning in LTE networks", *Informatica (Ljublj.)*, vol. 38, no. 3, pp. 135-143, 2014.
3. Evgen Benedik, Barbara Koroušič-Seljak, Marjan Simčič, Irena Rogelj, Borut Bratanič, Eric L. Ding, Rok Oreš, Nataša Fidler Mis, "Comparison of paper- and web-based dietary records: a pilot study", *Ann. nutr. metab.*, vol. 64, no. 2, pp. 156-166, 2014.
4. Mojca Bizjak, Zala Jenko Pražnikar, Barbara Koroušič-Seljak, "Development and validation of an electronic FFQ to assess food intake in the Slovene population", *Public health nutr. (Wallingford)*, vol. 17, iss. 8, pp. 1729-1737, 2014.
5. Cirila Hlastan-Ribič, Jožica Maučec Zakotnik, Barbara Koroušič-Seljak, Rok Poličnik, Urška Blaznik, Nataša Fidler Mis, Ivan Eržen, Chen Ji, Francesco P. Cappucio, "Estimation of sodium availability in food in Slovenia, results from household food purchase data from 2000 to 2009: rezultati iz raziskave o porabi živil v gospodinjstvih od leta 2000 do leta 2009", *Zdravstveno varstvo*, vol. 53, no. 2, pp. 209-219, 2014.
6. Uroš Kač, Franc Novak, "Practical considerations in oscillation based test of SC biquad filters", *Inf. technol. valdyn.*, vol. 43, no. 1, pp. 28-36, 2014.
7. Nada Rotovnik-Kozjek, Barbara Koroušič-Seljak, "Adult cancer patients on home parenteral nutrition in Slovenia: data analysis by the Clinical Nutrition Unit of the Institute of Oncology in Ljubljana, in the period 2008-2012: analiza podatkov Enote za klinično prehrano Onkološkega inštituta v Ljubljani, v obdobju 2008-2012", *Zdrav Vestn (Tisk. izd.)*, vol. 83, no. 3, pp. 232-239, mar. 2014.
8. Vida Vukašinović, Jurij Šilc, Riste Škrekovski, "Modeling acquaintance networks based on balance theory", *Int. J. Appl. Math. Comput. Sci.*, vol. 24, no. 3, pp. 683-696, 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Domen Butala, Dejan Velušček, Gregor Papa, "Empirical convergence analysis of genetic algorithm for solving unit commitment problem", In: *Bioinspired optimization methods and their applications: proceedings of the Student Workshop on Bioinspired Optimization Methods and their Applications - BIOMA 2014, 13 September 2014, Ljubljana, Slovenia*, Student Workshop on Bioinspired Optimization Methods and their Applications - BIOMA 2014, 13 September 2014, Ljubljana, Jurij Šilc, ed., Aleš Zamuda, ed., Ljubljana, Jožef Stefan Institute, 2014, pp. 127-140.
2. Nejc Cvörnjek, Miran Brezočnik, Timotej Jagrič, Gregor Papa, "Comparison between single and multi objective genetic algorithm approach for optimal stock portfolio selection", In: *Bioinspired optimization methods and their applications: proceedings of the Student Workshop on Bioinspired Optimization Methods and their Applications - BIOMA 2014, 13 September 2014, Ljubljana, Slovenia*, Student Workshop on Bioinspired Optimization Methods and their Applications - BIOMA 2014, 13 September 2014, Ljubljana, Jurij Šilc, ed., Aleš Zamuda, ed., Ljubljana, Jožef Stefan Institute, 2014, pp. 15-25.
3. Gašper Kojek, Anton Biasizzo, Franc Novak, "Implementation of PCI express interface on FPGA device using partial reconfiguration", In: *Conference 2014, proceedings*, 50th International Conference on Microelectronics, Devices and Materials, October 8 - October 10, 2014, Ljubljana, Slovenia, Marko Topič, ed., Polona Šorli, ed., Izток Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2014, pp. 169-172.
4. Matej Kristan, Janez Perš, Vildana Sulić Kenk, Stanislav Kovačič, "A graphical model for rapid obstacle image-map estimation from unmanned surface vehicles", In: *ACCV'14*, [S. l., s. n.], 2014, pp. 1-16.
5. Miha Ristič, Franc Novak, "Decision support in emergency call service", In: *Interakcija človek-računalnik v informacijski družbi: zbornik 17. mednarodne multikonference Informacijska družba - IS 2014, 8. oktober 2014, [Ljubljana, Slovenia]: zvezek H: proceedings of the 17th International Multiconference Information Society - IS 2014, October 8th, 2014, Ljubljana, Slovenia: volume H*, Franc Novak, ed., et al, Ljubljana, Institut Jožef Stefan, 2014, pp. 26-29.
6. Polona Tomašič, Gregor Papa, Martin Žnidaršič, "Automated slogan production using a genetic algorithm", In: *Bioinspired optimization methods and their applications: proceedings of the Student Workshop on Bioinspired Optimization Methods and their Applications - BIOMA 2014, 13 September 2014, Ljubljana, Slovenia*, Student Workshop on Bioinspired Optimization Methods and their Applications - BIOMA 2014, 13 September 2014, Ljubljana, Jurij Šilc, ed., Aleš Zamuda, ed., Ljubljana, Jožef Stefan Institute, 2014, pp. 55-66.
7. Polona Tomašič, Martin Žnidaršič, Gregor Papa, "Implementation of a slogan generator", In: *Proceedings, The Fifth International Conference on Computational Creativity, ICC3 2014, June 9-13, 2014 Ljubljana, Slovenia*, Simon Colton, ed., et al, Ljubljana, Institut Jožef Stefan, 2014, 4 pp..

## PATENT APPLICATION

1. Gregor Papa, Barbara Koroušič Seljak, Marko Pavlin, *Device and method for acquisition and transfer of signals*, GB1407135.1, Intellectual Property Office, 23.4.2014.

## MENTORING

1. Lucas Benedičič, *Optimization and parallelization methods for the design of next-generation radio networks*: doctoral dissertation, Ljubljana, 2014 (mentor Peter Korošec; co-mentor Tomaž Javornik).
2. Miha Ristič, *Improvement of user interface for police emergency call service*: master's thesis, Ljubljana, 2014 (mentor Franc Novak).
3. Jakob Bartolj, *Multicore processors in mobile devices*: master's thesis, Koper, 2014 (mentor Jurij Šilc).
4. Domen Butala, *Solving unit commitment problem with a genetic algorithm*: master's thesis, Ljubljana, 2014 (mentor Dejan Velušček; co-mentors Gregor Papa, Sabrina Guettes).
5. Blažka Hunski, *A polyhedral approach to mixed-integer linear programming and its application in dietetics*: master's thesis, Ljubljana, 2014 (mentor Marko Petkovšek; co-mentor Barbara Koroušič Seljak).







labeled data. We joined the Human Brain Project (FET Flagship), where we take part in the development of the Medical Informatics Platform. The platform will enable the analysis of large quantities of data routinely collected in hospitals for diagnostic purposes. To this end, we are developing methods for rule-based clustering, based on subgroup discovery and predictive clustering, which produce understandable cluster descriptions.

In the area of **computational creativity**, the developed banded-matrix approach to compound sentence ideation from two different corpora was evaluated and compared to other fictional narrative ideation approaches. In col-

laboration with the XLAB company we have developed a methodology for the automatic generation of slogans that is based on a combination of methods from computational linguistics, semantic resources and genetic algorithms.

We are active in the FP7 project MUSE (Machine Understanding for interactive Storytelling) in the area of the computer understanding of natural language, the goal of which is to convert text into a 3D animation. Since 2012 we are involved in the FP7 project PROSECCO, whose goal is the promotion of activities in the area of computational creativity. Since 2013 we have been collaborating in two computational creativity projects: ConCreTe (Concept Creation Technologies) and WHIM (The What-If Machine); the latter was evaluated as excellent at its first project review. In 2014 we organized the Fifth International Conference on Computational Creativity (ICCC 2014) in Ljubljana, and the Seventeenth International Conference on Discovery Science (DS 2014) in Bled, which attracted about 100 participants each.

In the area of **text and web mining and heterogeneous information network analysis** we successfully concluded the FET project FOC (Forecasting Financial Crises) with an excellent final evaluation. We started work on two new projects, SIMPOL (Financial Systems Simulation and Policy Modelling)

and MULTIPLEX (Foundational Research on MULTilevel comPLEX networks and systems).

The SIMPOL project aims to support decision makers and regulators in policy modeling and impact analysis, with the emphasis on financing sustainable and environmentally friendly projects. We have developed a knowledge-sharing platform to support data collection and analysis. The knowledge representation is based on graphs and on Semantic Web principles. The data model is stored in Neo4j, a high-performance, non-SQL database designed

to efficiently manipulate and query graphs. We have implemented the web portal <http://simpol.ijs.si/>, which uses Neo4j as its back-end. The portal supports activities to build socio-economic networks: the overview, selection and inspection of existing networks in the database, the extraction of networks from open data, the import/export interface to a crowd-sourcing platform, the monitoring of news and blogs, and social-media monitoring.

The goal of MULTIPLEX is the development of a mathematical framework of complex networks and algorithms aimed at establishing a theoretical basis for the understanding, prediction and, possibly, the control of complex

systems. Our role is to extract multilevel networks from textual data streams, i.e., news, blogs and Twitter. From tweets about environmental issues, we extracted a re-tweet network, assigned influence to the actors and sentiment to their tweets, and computed major network communities. Based on the sentiment assigned to the communities, we analyzed their leanings towards various environmental issues. From financial news, we created time-varying, co-occurrence networks for 50 countries, and compared them to financial, trade, and geographical networks. It turns out that the news mostly reflects geographical proximity. However, positive-sentiment news items are the most similar to trade networks.

In the area of **language technologies and digital humanities** we work mostly on producing language resources and methods to annotate text with linguistic information, with a focus on the Slovene language. In 2014 we started work on the national research project JANES (Resources, Tools and Methods for Research of Non-standard Internet Slovene), <http://nl.ijs.si/janes/>, which is led by the Dept. of Translation at the Faculty of Arts at the University of Ljubljana. We have compiled slWaC 2.0, a new corpus of Slovene gathered from Web documents, containing over one billion words. We have also developed a tool, called TweetCaT, for collecting tweets in a given language and a method using character-based statistical machine translation to normalize non-standard language. With these tools we produced the first large, linguistically annotated corpus of Slovene tweets, which contains over 35 million words. We have also started work on extracting Slovene user comments, forums and blogs from the Web.

The recently concluded IMP project, <http://nl.ijs.si/imp/>, produced a large set of resources of historical Slovene, including a digital library, dictionary and corpus, all available on the Web. We conducted a study to analyze

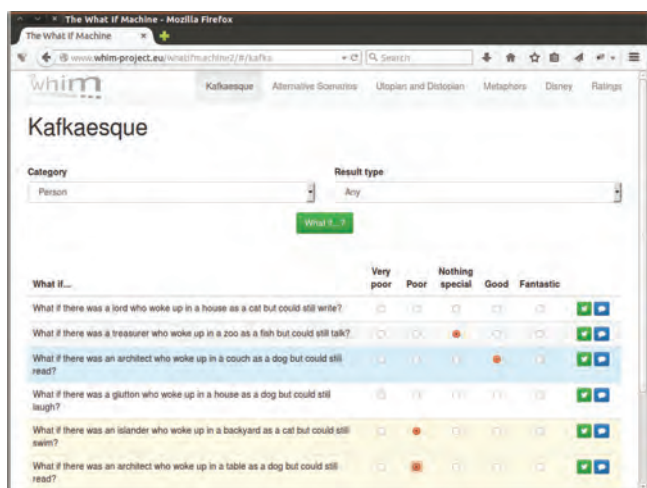


Figure 2: Web interface of "The What-if machine" and its components for crowd-sourcing evaluation.

**The "NoiseRank" method for the detection and ranking of noise and anomalies in data, was recognized as an outstanding scientific achievement by the Scientific Research Council for Engineering Sciences of the ARRS and was presented at the event "Excellent in Science 2013" as part of the 9th Slovenian Innovation Forum 2014.**

the users' experience with these resources, which showed that most users (predominantly teachers and students) consider the resources important for their work and for Slovene linguistics in general; useful suggestions for improvements were gathered, too. We also continued our cooperation with the Slovenian Academy of Sciences and Arts on producing their Web-based Slovene Biographical Lexicon(s).

We were active in developing the concept of a planned new dictionary of the Slovene language, in advocating open access to language resources taken as scientific data, and in establishing the Slovene research infrastructure CLARIN.SI. This infrastructure is now organized as a consortium with, currently, eleven partners: three Slovenian universities (Ljubljana, Maribor, Primorska), three research institutes (SRC SASA, JSI, INZ), as well as societies (SDJT, Trojina, DZDR) and companies (Amebis, Alpineon) dealing with language technologies and resources. The CLARIN.SI infrastructure now meets the organizational and technical criteria so that it could become a member of the European CLARIN ERIC in 2015, with Slovenia having a stable and permanent repository for language resources and language-technology-related web services.

In October we organized, in the scope of the JSI Information Society Meta-Conference, the 9th conference on Language Technologies. These biennial conferences have become the main forum for the presentation of research on language technologies and related fields in Slovenia, as well as in Croatia. The proceedings of the 2014 conference contain two invited lectures and 29 reviewed regular papers with 180 pages.

We continued our work in the context of the ESF network NetWordsS (European Network on Word Structure), in the COST action PARSEME (Parsing and Multi-word Expressions), and started work in the context of two bilateral projects, one with Croatia and the other with Serbia. We collaborated in the work of the Slovene Institute for Standardization as the Slovene representatives in ISO/TC37/SC4 (Terminology and Other Language and Content Resources / Language Resources Management) by reviewing, translating and approving Slovene standards from this field. For the Slovenian Ministry of Culture we helped in preparing the Action Plan for the National Program for Language Policy 2014-2018.

In the area of **decision support**, our long-term goal is to develop methods and techniques for decision modeling, support them with software and integrate them with data-mining systems. In 2014 we focused on extending the qualitative, multi-attribute method DEX in the directions of including numeric criteria, using probabilistic value distributions and considering relationally-defined decision alternatives, as well as developing corresponding software tools. We updated our computer program for multi-attribute modeling DEXi and added features for the visualization of utility functions. We investigated the potential of the aggregation-disaggregation methods UTA and ACUTA for the representation of DEX utility functions. In the application area, we successfully completed two main projects: FP7 FIRST, in which we developed a system for the assessment of bank reputational risk, and the Slovene project OVJE, in which we developed decision models and a decision-support system for the assessment of the sustainability of electric energy production in Slovenia until 2030. Other applications include emergency management, strategic management in companies, decision support in protected areas, and the production of game devices.

Within the EVADIFF project (Evaluation et de développement et modèles outils d'aide à la décision utilisés pour la Prévention des pollutions diffuses par les produits phytopharmaceutiques), commissioned by ARVALIS Institut du Vegetal, France, we completed the development of a decision-support system for the selection of mitigation measures for the protection of surface waters from pollution by phyto-pharmaceuticals. The system makes use of qualitative evaluation models based on expert knowledge and quantitative predictive models generated by data mining. After the integration, customization and user training, the system will be deployed within ARVALIS during 2015.

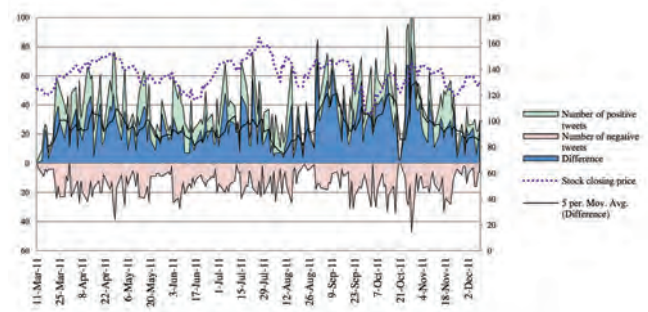


Figure 3: Visual representation of the sentiment of Twitter messages discussing stocks of the Baidu company.

**In 2014, the department organized three international conferences: the Fifth International Conference on Computational Creativity (ICCC 2014), the Seventeenth International Conference on Discovery Science (DS 2014), and the Ninth Language Technologies Conference at the Information Society Multiconference (LT@IS 2014).**

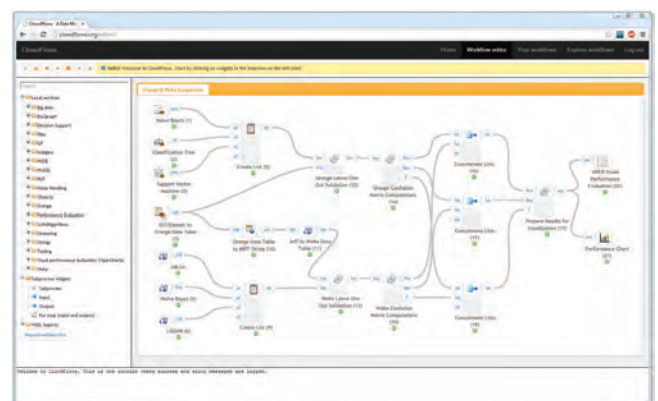


Figure 4: A typical data-mining workflow in the web-based CloudFlows platform.

## Some outstanding publications in the last year

1. Ikonomovska, E., Gama, J., Džeroski, S.: Online tree-based ensembles and option trees for regression on evolving data streams. *Neurocomputing*, ISSN 0925-2312, 2015, vol. 150, part. 150, pp. 458-470, doi: 10.1016/j.neucom.2014.04.076.
2. Levatić, J., Kocev, D., Džeroski, S.: The importance of the label hierarchy in hierarchical multi-label classification. *Journal of intelligent information systems*, ISSN 0925-9902, [in press] 2014, 25 pp., doi: 10.1007/s10844-014-0347-y.
3. Miljković, D., Depolli, M., Stare, T., Mozetič, I., Petek, M., Gruden, K., Lavrač, N.: Plant defence model revisions through iterative minimisation of constraint violations. *International journal of computational biology and drug design*, ISSN 1756-0756, 2014, vol. 7, no. 1, pp. 61-79, doi: 10.1504/IJCBD.2014.058588.
4. Panov, P., Soldatova, L. N., Džeroski, S.: Ontology of core data mining entities. *Data mining and knowledge discovery*, ISSN 1384-5810, [in press] 2014, 44 pp., doi: 10.1007/s10618-014-0363-0.
5. Piškorec, M., Antulov-Frantulin, N., Kralj Novak, P., Mozetič, I., Grčar, M., Vodenska I., Šmuc, T.: Cohesiveness in Financial News and its Relation to Market Volatility, *Scientific Reports* 4, 5038-1-8, 2014.
6. Popovič, M., Štefančič, H., Sluban, B., Kralj Novak, P., Grčar, M., Mozetič, I., Puliga, M., Zlatič, V.: Extraction of Temporal Networks from Term Co-occurrences in Online Textual Sources, *PLoS ONE* 9(12), e99515, 2014.
7. Ramšak, Ž., Baebler, Š., Rotter, A., Korbar, M., Mozetič, I., Usadel, B., Gruden, K.: GoMapMan: integration, consolidation and visualisation of plant gene annotations within the MapMan ontology, *Nucleic Acids Research* 42(D1), D1167-D1175, 2014.
8. Sluban, B., Gamberger, D., Lavrač, N.: Ensemble-based noise detection: noise ranking and visual performance. *Data mining and knowledge discovery*, ISSN 1384-5810, 2014, vol. 28, no. 2, pp. 265-303.
9. Smailović, J., Grčar, M., Lavrač, N., Žnidaršič, M.: Stream-based active learning for sentiment analysis in the financial domain. *Information sciences*, ISSN 0020-0255, 2014, vol. 285, pp. 181-203, doi: 10.1016/j.ins.2014.04.034.
10. Vavpetič, A., Podpečan, V., Lavrač, N.: Semantic subgroup explanations. *Journal of intelligent information systems*, ISSN 0925-9902, 2014, vol. 42, no. 2, pp. 233-254, doi: 10.1007/s10844-013-0292-1.

## Awards and appointments

1. Nejc Trdin: Best Doctoral Consortium Contribution at the Conference 17th IFIP WG 8.3 DSS 2014, Paris, France, New Generation Platform for Multi-Criteria Decision Making with Method DEX.
2. Nejc Trdin: International Postgraduate School's Recognition, Applicant: Dean and President of Jožef Stefan International Postgraduate School
3. Borut Sluban: Recognition for outstanding scientific achievement in 2013 by the ARRS as part of the 9th Slovenian Innovation Forum, 13. 11. 2014, "NoiseRank method for detecting anomalies in the data".

## Organization of conferences, congresses and meetings

1. ICCV 2014 - International Conference on Computational Creativity, Ljubljana, Slovenia, 10-13 June 2014
2. "The 17th International Conference on Discovery Science", Bled, Slovenia, 8-10 October 2014
3. "The 25th International Conference on Algorithmic Learning Theory", Bled, Slovenia, 8-10 October 2014
4. Project meeting of European project MAESTRA, Ljubljana, Slovenia, 3-5 February 2014
5. Project meeting of European project MAESTRA, Bled, Slovenia, 7 October 2014

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## INTERNATIONAL PROJECTS

1. EVADIFF; Evaluation of Existing Models and Development of New Decision-making Tools to prevent Diffuse Pollution caused by Plant Protection Products  
Prof. Marko Debeljak  
ARVALIS - Institut du Végétal
2. Training on Multi-Criteria Decision Analysis (MCDA)  
Prof. Marko Bohanec  
Honda R&D Europe (Deutschland) GmbH
3. 7FP - SUMO; Supermodeling by Combining Imperfect Models  
Prof. Sašo Džeroski  
European Commission
4. 7FP - REWIRE; Rehabilitative Wayout In Responsive home Environments  
Prof. Sašo Džeroski  
European Commission
5. 7FP - FOC-II; Forecasting Financial Crises

6. 7FP - MUSE; Machine Understanding for interactive StoryTElling  
Prof. Nada Lavrač  
European Commission
7. 7FP - PROSECCO; Promoting the Scientific Exploration of Computational Creativity  
Prof. Nada Lavrač  
European Commission
8. 7FP - ConCreTe; Concept Creation Technology  
Prof. Nada Lavrač  
European Commission
9. 7FP - SIMPOL; Financial Systems Simulation and Policy Modelling  
Dr. Igor Mozetič  
European Commission
10. 7FP - MULTIPLEX; Foundational Research on Multilevel Complex Networks and Systems  
Dr. Igor Mozetič  
European Commission

11. 7FP - WHIM; The What-If Machine  
Prof. Nada Lavrač  
European Commission
12. 7FP - MAESTRA; Learning from Massive, Incompletely Annotated, and Structured Data  
Prof. Sašo Džeroski  
European Commission
13. 7FP - DECATHLON; Development of Cost efficient Advanced DNA-based methods for specific Traceability issues and High Level On-site applicatioNs  
Prof. Marko Bohanec  
European Commission
14. 7FP - HBP; The Human Brain Project  
Prof. Sašo Džeroski  
European Commission
15. COST IC1002; MUMIA; Multilingual and Multifaceted Interactive Information Access  
Dr. Igor Mozetič  
COST Office
16. PARSEME: PARSing and Multi-Word Expressions. Towards Linguistic Precision and Computational Efficiency in Natural Language Processing  
Asst. Prof. Tomaž Erjavec  
COST Office
17. Constructing a Bilingual Lexicon of Closely Related Languages From Existing Language Resources  
Asst. Prof. Tomaž Erjavec  
Slovenian Research Agency
18. The Construction of Corpora and Lexica of Nonstandard Serbian and Slovenian  
Asst. Prof. Tomaž Erjavec  
Slovenian Research Agency
2. Development and Applications of New Semantic Data Mining Methods in Life Sciences  
Prof. Nada Lavrač
3. Growth and Defense Trade-Offs in Multitrophic Interaction between potato and its Two Major Pests  
Prof. Nada Lavrač
4. The Leading Humanists in the Slovenian Territory between the 16th and mid-19th Centuries and their Social and Cultural Environment  
Asst. Prof. Tomaž Erjavec
5. Slovenian Literature in Unknown Early Modern Manuscripts: Information-Technology Aided Analyses and Scholarly Editions  
Asst. Prof. Tomaž Erjavec
6. Resources, Tools and Methods for the Research of Nonstandard Internet Slovene  
Asst. Prof. Tomaž Erjavec
7. Ecological Restoration of Natural Disturbances in Forests  
Prof. Marko Debeljak
8. Workflows in the Cloud  
Dr. Darko Cherepnalkoski
9. Sentiment Analysis  
Dr. Matjaž Juršič
10. The European Network on Word Structure  
Asst. Prof. Tomaž Erjavec
11. The Fifth International Conference on Computational Creativity - ICC3 2014, 10-13 June 2014, Ljubljana, Slovenia  
Prof. Nada Lavrač
12. DS/ALT 2014 - The 17th International Conference on Discovery Science and The 25th International Conference on Algorithmic Learning Theory  
Prof. Sašo Džeroski

## RESEARCH PROGRAM

1. Knowledge Technologies  
Prof. Nada Lavrač

## R & D GRANTS AND CONTRACTS

1. Integrative Research of Sexual Dimorphism Evolution  
Prof. Sašo Džeroski

## NEW CONTRACTS

1. Sustainability Appraisal of Energy Policy Development in Slovenia by 2030 with the Emphasis on Nuclear Option  
Prof. Marko Bohanec  
Gen Energija, d. o. o.
2. Shallow Semantic Analyses for Selected European Languages  
Dr. Igor Mozetič  
Gama System, d. o. o.

## VISITORS FROM ABROAD

1. Prof. Werner Dubitzky, University of Ulster, School of Biomedical Sciences, Coleraine, Ireland, 9–12 January 2014
2. Prof. Jaakko Hollmen, Aalto University School of Science, Department of Information and Computer Science, Aalto, Finland, 6–12 January 2014
3. Dr. Richard Wheeler, University of Edinburgh, Edinburgh, Scotland, 26 January–2 February 2014
4. Dr. Ivica Dimitrovski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, University of Skopje, Skopje, Macedonia, 19 January–8 February 2014
5. Prof. Johannes Fuernkranz, Technical University Darmstadt, Darmstadt, Germany, 18–19 March 2014
6. Dr. Gjorgji Madjarov, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, University of Skopje, Skopje, Macedonia, 3–5 February 2014
7. Prof. Dejan Gjorgjevik, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, University of Skopje, Skopje, Macedonia, 3–5 February 2014
8. Prof. Michelangelo Ceci, Università degli Studi di Bari "Aldo Moro", Bari, Italy, 2 February–2 March 2014
9. Dr. Nikola Ljubešić, University of Zagreb, Zagreb, Croatia, 5 March–20 May 2014
10. Benoit Real, ARVALIS-Institut du végétal, Paris, France, 10–13 March 2014
11. Jonathan Marks-Perreau, ARVALIS-Institut du végétal, Paris, France, 10–13 March 2014
12. Ruslan Miniakhmetov, Southern Ural State University, Chelyabinsk, Russia, 24 March–12 June 2014
13. Jozef Mišutka, University of Prague, Prague, Czech Republic, 22–26 April 2014
14. Dr. Ivica Slavkov, Centre of Genomic Regulation, Barcelona, Spain, 10–18 May 2014
15. Dr. Dragan Gamberger, Ruder Bošković Institute, Zagreb, Croatia, 19 May 2014
16. Dr. Tomislav Šmuc, Ruder Bošković Institute, Zagreb, Croatia, 19 May 2014
17. Dr. Simon Colton, University of London, London, England, 9 June 2014
18. Dr. Tony Veale, University College Dublin, Dublin, Ireland, 9 June 2014
19. Prof. F. Amílcar Cardoso, Universidade de Coimbra, Coimbra, Portugal, 9 June 2014
20. Prof. Pablo Gervas, Universidad Complutense de Madrid, Madrid, Spain, 9 June 2014
21. Prof. Geraint Wiggins, Queen Mary University of London, London, England, 9 June 2014
22. Ian Gouldstone, London, England, 9 June 2014
23. Prof. Hannu Toivonen, University of Helsinki, Helsinki, Finland, 9 June 2014
24. Benoit Real, ARVALIS-Institut du végétal, Paris, France, 25–29 August 2014
25. Jonathan Marks-Perreau, ARVALIS-Institut du végétal, Paris, France, 25–29 August 2014
26. Matej Durco, Institute for Corpus Linguistics and Text Technology, Austria, 8–10 October 2014
27. Maja Popović, Language Technology Lab, Germany, 8–12 October 2014
28. Dr. Ivica Dimitrovski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, University of Skopje, Skopje, Macedonia, 5–7 October 2014
29. Dr. Ivica Dimitrovski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, University of Skopje, Skopje, Macedonia, 10–11 October 2014
30. Prof. Stefano Battison, University of Zurich, Switzerland, 22–23 October 2014
31. Eneldo Loza Mencia, TU Darmstadt, Knowledge Engineering Group, Darmstadt, Germany, 10–31 October 2014
32. Dr. Tomislav Šmuc, Ruder Bošković Institute, Zagreb, Croatia, 11 December 2014
33. Dr. Matej Mihelčić, Ruder Bošković Institute, Zagreb, Croatia, 11 December 2014
34. Dr. Ivan Ivek, Ruder Bošković Institute, Zagreb, Croatia, 11 December 2014

## STAFF

### Researchers

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  8. Asst. Prof. Martin Znidarič
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  10. Dr. Darko Cherepnalkoski



11. Dr. Matjaž Jursič  
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2. Senja Pollak, *Semi-automatic domain modeling from multilingual corpora*: doctoral dissertation, Ljubljana, 2014 (mentor Špela Vintar; co-mentor Paola Velardi).
3. Borut Sluban, *Ensemble-based noise and outlier detection*: doctoral dissertation, Ljubljana, 2014 (mentor Nada Lavrač).
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# DEPARTMENT OF INTELLIGENT SYSTEMS

E-9

*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 and multi-agent systems, and language and speech technologies. The department collaborates closely with the Faculty of Computer and Information Science of the University of Ljubljana on the joint research program "Artificial Intelligence and Intelligent Systems", led by Prof. Ivan Bratko. The department also closely collaborates with industry and significantly contributes to the employment of intelligent systems in products and services.*

Intelligent systems simulate intelligence so that a typical user perceives them as truly intelligent. In reality, these systems use complex mechanisms and implement them on digital computers to imitate human behavior as well as possible, exploiting raw, exponentially growing computer power. This field is improving greatly worldwide.

**Ambient intelligence** is a research area aiming to introduce technology into our everyday environment in a friendly way that is undemanding for the user. The two key topics of ambient intelligence we work on are e-health and the smart home. On the topic of e-health, our focus in the past year, was the FP7 project COMMODITY12, which telemonitors diabetes patients. The department's main task in the project is the analysis of patients' lifestyles using sensors in a smartphone and on a chest strap. We developed a method that first automatically recognizes which of these devices a patient carries, then it normalizes the orientation of the phone and detects in which pocket it is carried, and finally invokes the appropriate models to recognize the patient's activity and estimates his/her energy expenditure. This method achieves results comparable to those that can be achieved with dedicated sensors. We started the AAL project Fit4Work, whose goal is to detect mental and physical stress in older workers, and help them with relaxation and physical exercises. We have begun developing methods that recognize mental stress from the behavior of the worker as measured with sensors in his/her smartphone and wristband, and from voice. The department is also a part of the Slovenian team in the XPrize Tricorder competition with prize money of 10 million dollars. The department's role is

to develop a method that comes up with an accurate tentative diagnosis (later confirmed by a dedicated diagnostic device) by asking as few questions as possible. Our team was ranked among the ten finalists among the more than 300 registered. On the topic of the smart home, we continued working on the Intelligent E-doorman System developed in collaboration with the Development Center Intech-Les, upgrading it into the QuGuard platform. We improved the intruder alert by introducing face detection, and increased the extensibility of the platform, since our goal is to use it in all upcoming smart-home applications. The first of them will be developed in the Horizon 2020 project In Life, which was accepted last year. This project will attempt to deploy various systems for elderly care in real life.

**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 multiobjective optimization and their speedup, and apply these algorithms in engineering design and optimization problems. In doctoral research projects, we visualized 3D empirical attainment functions in multiobjective optimization using three methods, i.e., slicing, maximum intensity projection and direct volume rendering, and developed a two-level multiobjective optimization algorithm for discovering optimal driving strategies for intelligent vehicles that optimizes three criteria: travelling time, fuel consumption and driving comfort. The key area of testing and transferring our methods to practice is production-process optimization. In collaboration with the University of Nova Gorica, the Institute of Metals and Technology, Ljubljana, and the Štore Steel company, we completed an applied research project on simulation and optimization of casting, rolling and heat-treatment processes for the competitive production of topmost steels. As a result, we developed a web application VizEMO-Steel that is used by the Štore Steel company to optimize the continuous steel casting process and visualize the results. In addition, with the University of Nova Gorica and the Institute of Metals and Technology, Ljubljana, we completed a research project on the advanced



Head:  
**Prof. Matjaž Gams**

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**The Department of Intelligent Systems was ranked among the best 10 groups out of 300 registered at the XPrize Tricorder competition, where teams vie for 10 million dollars in prizes for the best consumer medical diagnostic devices.**

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**For the Štore Steel company we developed a web application VizEMO-Steel that supports the optimization of a continuous steel casting process and the visualization of the results.**

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modelling and simulation of liquid-solid processes called **SMACS**. Using the multiobjective optimization methods, we minimized the concentration and structural inhomogeneities in the solidified material by influencing the cooling process dynamics. We continued our research within the **COPCAMS** project, approved for funding under the Artemis call. Together with the Slovenian industrial partner Kolektor and international partners we are developing production quality-control procedures that are based on computer vision, machine learning and optimization.

In the field of **agent and multi-agent systems** the two key research areas are smart autonomous systems, such as smart city and smart home, and the strategic behaviour analysis of a group of agents. The European project **ACCUS** is aimed at developing an integration and coordination platform for urban systems to build applications across urban systems, providing adaptive and cooperative control for urban subsystems, and optimizing the combined performance. The platform currently optimizes electrical consumption in smart houses, production in

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**The OpUS intelligent-home automation system reduces energy consumption by 5 to 20%.**

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thermal power plants, traffic flow and thus affects the outside parameters, such as air quality. The smart-city control continuously monitors the conditions in the city and, for example, when a warning about high air pollution is triggered it decides to lower the traffic flow, the energy consumption in

residential areas and production in the local thermal power plant. The monitoring system in several time steps verifies the effects of the control actions and, if required, sends additional corrections until an adequate level of air quality is achieved. A similar system is studied within the national project **OPUS**, where the focus is on the development of smart home automation services. The aim is to apply advanced machine learning and optimization methods in order to generate real-time control strategies that increase the users' comfort and at the same time decrease operational costs of the smart home. We experimentally demonstrated that it is possible to achieve energy savings without reducing comfort. In a similar project we tried to improve the user comfort through the regulation of temperature. The observed improvements were significant, mostly due to the successful predictions of home occupancy. Additional improvements were achieved when applying learning algorithms to the heat pumps. The controller learns the user's behaviour and formulates a strategy for water heating during periods of cheaper electricity and at the same time it lowers the temperature of the stored water during days of lower consumption. In the area of agent-based strategic-behaviour analysis, we continued the work performed on the **EUSAS** project, which was focused on the development of a new approach to mission training for low-level units (security, police force, etc.) facing asymmetric threats in an urban environment. We developed algorithms and tools that can be used to discover the common-agent strategy by knowing only 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. Meaningful behaviour patterns are later used in behaviour cloning, where software agents reproduce the observed human behaviour in a specific domain.

In the field of **speech and language technologies** we work on speech synthesis, the semantic analysis of text and question answering. Together with the Amebis company, we developed a new speech synthesizer for Slovene. Both the comprehensibility and naturalness of the synthesized speech have been greatly improved. Special attention is paid to the requirements of elderly, handicapped, visually impaired people and to apply our solutions to smart

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**The new speech synthesizer for Slovene greatly improves the comprehensibility and naturalness of synthesized speech.**

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devices and homes. In the past year, we manually improved a phonetically rich and balanced speech database for corpus-based speech synthesis by automatic speech-recognition methods. The speech database was recorded in cooperation with the national television and radio, RTV Slovenia. We started to develop a free text-to-speech synthesis service for mobile devices.

For purposes of the JSI we developed an adapted version of the virtual assistant, Robi, which enables employees and visitors to quickly and easily find information regarding the JSI and also provides a rich set of additional applications that offer various new functionalities (employee phone book, infrastructure malfunction reporting, etc.).

The focus points of the research and developmental potential of the department are also being expressed in successfully developed, integrated and deployed solutions, available on major digital platforms and available to a wide population of users. The methods used in typical applied projects combine the procedures of intelligent agents, statistical methods and machine learning, and serve as a basis for user interfaces on smart phones, pads or desktop computers. The projects' services are developed for all key mobile platforms: Android, iOS, Windows 8 and BlackBerry, and through classic web clients.

From 13 to 17 September 2014, the **13th International Conference on Parallel Problem Solving from Nature – PPSN 2014** was held at the Ljubljana Exhibition and Convention Centre. It was organized by the Department of Intelligent Systems and the Computer Systems Department of the Jožef Stefan Institute. This meeting is devoted to the methods of natural computing, which take inspiration from biological, ecological, physical and social systems, and are used in optimization and data mining. The conference was attended by 180 participants from 28 countries, the authors presented 90 papers, and the proceedings were published by Springer.

From 6 to 10 October 2014, the **17th International Multiconference Information Society – IS 2014** ([is.ijs.si](http://is.ijs.si)) took place at the Jožef Stefan Institute. It consisted of twelve independent conferences with around 400 participants presenting approximately 200 papers. Four conference awards were given: for lifetime achievements (“Donald Michie and Alan Turing” award) to Prof. Janez Grad, for current achievements in the field of information society to Prof. Janez Demšar, and the information strawberry and lemon for the best and worst public information-society services.

The department registered two patent applications and was awarded a patent.

### Some outstanding publications in the last year

1. Dovgan, E., Javorski, M., Tušar, T., Gams, M., Filipič, B.: Discovering driving strategies with a multiobjective optimization algorithm. *Applied Soft Computing*, 16 (2014), 1, 50–62
2. Gjoreski, H., Gams, M., Luštrek, M.: Context-based fall detection and activity recognition using inertial and location sensors. *Journal of Ambient Intelligence and Smart Environments*, 6 (2014), 4, 419–433
3. Kaluža, B., Cvetkovič, B., Dovgan, E., Gjoreski, H., Mirchevska, V., Gams, M., Luštrek, M.: A Multiagent care system to support independent living. *International Journal on Artificial Intelligence Tools*, 23(2014), 1, 1440001-1–1440001-30
4. Mlakar, M., Tušar, T., Filipič, B.: Comparing solutions under uncertainty in multiobjective optimization. *Mathematical Problems in Engineering*, 2014, doi:10.1155/2014/817964
5. Tušar, T., Filipič, B.: Visualizing exact and approximated 3D empirical attainment functions. *Mathematical Problems in Engineering*, 2014, doi: 10.1155/2014/569346
6. Vidulin, V., Bohanec, M., Gams, M.: Combining human analysis and machine data mining to obtain credible data relations. *Information Sciences*, 288(2014), 254–278
7. Zupančič, D., Luštrek, M., Gams, M.: Multi-agent architecture for control of heating and cooling in a residential space. *The Computer Journal*, 2014, doi: 10.1093/comjnl/bxu058

### Awards and appointments

1. Hristijan Gjoreski: Award for presenting scientific achievements with scientific quality and practical usage, Ljubljana, 6th Jožef Stefan International Postgraduate School Students' Conference, Recognizing human activities and detecting falls in real-time
2. Hristijan Gjoreski, Rok Piltaver: ECCAI Travel Award 2014, Prague, Czech Republic, European Coordinating Committee for Artificial Intelligence (ECCAI), Multi-objective learning of hybrid classifiers
3. Anton Gradišek: Fulbright scholarship for work in the USA, United States Department of State Bureau of Educational and Cultural Affairs
4. Mitja Luštrek, Matjaž Gams, Anton Gradišek, Maja Somrak: Reaching the final of Qualcomm Tricorder Xprize, Chicago, ZDA, X Prize Foundation for an automatic non-invasive health, delivering diagnostics HealthStation Home as part of the Mesi Simplifying diagnostics team

### Organization of conferences, congresses and meetings

1. 24th Slovene Workshop on Nature-Inspired Algorithms, AVN, Ljubljana, Slovenia, 23 May 2014
2. Student Workshop at the Genetic and Evolutionary Computation Conference, GECCO 2014, Vancouver, Canada, 12 July 2014
3. 13th International Conference on Parallel Problem Solving from Nature, PPSN 2014, Ljubljana, Slovenia, 13–17 September 2014
4. 17th International Multiconference Information Society, IS 2014, Ljubljana, Slovenia, 6–10 October 2014; independent conferences:
  - Intelligent systems
  - Facing demographic challenges
  - Collaboration, software and services in information society
  - Cognitive sciences
  - Data mining and data warehouses
  - Education in information society
  - Robotics
  - Language technologies
  - 1st Student Computer Science Research Conference (StuCoSReC)
  - Human-computer interaction in information society
  - Environmental ergonomics & physiology

5. Chiron workshop: technology and cardiovascular health

## Patent granted

1. Matjaž Gams, Hristijan Gjoreski, Mitja Luštrek, Boštjan Kaluža, Method and system for context-based activity recognition, SI24356 (A), Urad RS za intelektualno lastnino, 28.11.2014.
2. Matjaž Gams, Tea Tušar, Darko Zadavec, Matej Horvat, System and method for continuous control and management of tablet manufacturing process, SI24243 (A), Urad RS za intelektualno lastnino, 30.5.2014.
3. Damjan Kužnar, Matjaž Gams, Domen Marinčič, Marko Lotrič, Klemen Čufar, Method for intelligent control of refrigeration systems of cooling devices, SI24163 (A), Urad RS za intelektualno lastnino, 28.2.2014.

## INTERNATIONAL PROJECTS

1. 7FP - Xperience; Robots Bootstrapped through Learning from Experience  
Prof. Matjaž Gams  
European Commission
2. 7FP - Commodity12; Continuous Multi-parametric and Multi-layered Analysis of Diabetes Type 1&2  
Dr. Mitja Luštrek  
European Commission
3. CIP Programme; EcoDots  
Dr. Mitja Luštrek  
European Commission
4. COST TD1405; ENJECT, European Network for the Joint Evaluation of Connected Health Technologies  
Božidara Cvetković, B. Sc.  
COST Office

## RESEARCH PROGRAM

1. Artificial Intelligence and Intelligent Systems  
Prof. Matjaž Gams

## R & D GRANTS AND CONTRACTS

1. Advanced Modelling and Simulation of Liquid-Solid Processes  
Prof. Bogdan Filipič
2. Simulation and Optimization of Casting, Rolling and Heat Treatment Processes for Competitive Production of Topmost Steels  
Prof. Bogdan Filipič
3. Open Communication Platform for Service Integration: CC OPCOMM  
Prof. Matjaž Gams
4. Research on Adaptive Predictive Domain Models  
Dr. Boštjan Kaluža
5. Optimizing the Management of Energy Efficient Smart Buildings  
Dr. Tomaž Šef
6. Adaptive Cooperative Control in Urban (sub) Systems  
Prof. Matjaž Gams

7. COgnitive & Perceptive CAMeras: COPCAMS  
Prof. Bogdan Filipič
8. DysLex: Universal Voice e-Reader for the Slovenian Language as a Personal Learning Tool for People with Dyslexia and Different Types of Visual Disturbances  
Dr. Tomaž Šef
9. Metis: e-Service for the Early Detection of Learning Issues  
Dr. Erik Dovgan
10. e-Xercise: Mobile Application to Monitor and Promote Exercise in Schoolchildren for More Effective Physical Education  
Dr. Mitja Luštrek
11. Self-management of Physical and Mental Fitness of Older Workers  
Dr. Mitja Luštrek

## NEW CONTRACTS

1. Critical Analysis and Evaluation of Multiobjective Optimization and Machine Learning Methods for Intelligent Home Services  
Dr. Tomaž Šef  
Robotina, d. o. o.
2. Analysis and Evaluation of Advanced Spoken Language Technologies for Smart Buildings  
Dr. Tomaž Šef  
Amebis, d. o. o., Kamnik
3. User-oriented Business Reporting  
Prof. Matjaž Gams  
Result, d. o. o.
4. Intelligent Methods for Prediction of Calibration Timing  
Prof. Matjaž Gams  
Špica International, d. o. o.
5. Analysis of Shopping Behavior of Customers in Online Stores  
Dr. Mitja Luštrek  
Creatim Ržišnik Perc, d. o. o.
6. Research of Intelligent Algorithms Applicability for Sensor Data Processing on Embedded Devices  
Prof. Matjaž Gams  
Elgoline, d. o. o.
7. Research of Intelligent Algorithms Applicability for Sensor Data Processing on Embedded Devices  
Prof. Bogdan Filipič  
Store Steel, d. o. o.

## VISITORS FROM ABROAD

1. William Vulgaire, University of Paris Sud XI, Paris, France, 14 April–28 June 2014
2. Marwan Belgueddab, University of Paris Sud XI, Paris, France, 2 June–1 September 2014
3. Guillaume Bizet, University of Paris Sud XI, Paris, France, 2 June–1 September 2014
4. Aurel Billet, University of Paris Sud XI, Paris, France, 2 June–1 September 2014
5. Thomas Villeboeuf, University of Paris Sud XI, Paris, France, 2 June–1 September 2014
6. Mukhiddin Yusupov, Czech Technical University, Electrical Engineering, Cybernetics and Artificial Intelligence, Prague, Czech Republic, 1 July–15 September 2014
7. Kerhoff Rutgerus Hendrikus, Utrecht University, Faculty of Science, Netherlands, 7 July–31 August 2014
8. Mario Konecki, Faculty of Organization and Informatics, Department of Theoretical and Applied Foundations of Information Sciences, Varaždin, Croatia, 13 July–30 November 2014
9. Eda Kalayci, Yildiz Technical University, Faculty of Electrical and Electronics, Computer Engineering Department, Turkey, 14 July–5 September 2014
10. Martin Gjoreski, Faculty of Computer Science and Engineering, Univerzitet Sv. Kiril in Metodij, Skopje, Macedonia, 1 October–31 December 2014

## STAFF

### Researchers

1. Prof. Ivan Bratko\*
2. Asst. Prof. Aleš Dobnikar\*
3. Prof. Bogdan Filipič
4. Prof. Matjaž Gams, Head

5. Dr. Mitja Luštrek
  6. Dr. Domen Marinčič\*
  7. Dr. Tomaž Šef
- Postdoctoral associates**
8. Dr. Erik Dovgan

9. Dr. Anton Gradišek
10. Dr. Matej Guid\*
11. Dr. Boštjan Kaluža
12. Dr. Violeta Mirchevska
13. Dr. Aleksander Pivk\*
14. Dr. Tea Tušar
15. *Dr. Vedrana Vidulin, on postdoctoral leave since 11. 03. 14*
- Postgraduates
16. Robert Blatnik, M. Sc.
17. Božidara Cvetković, B. Sc.
18. Tomaž Kompara\*, B. Sc.
19. Dr. Jana Krivec\*
20. *Damjan Kužnar\*, B. Sc., left, 30. 06. 14*
21. Miha Mlakar, B. Sc.
22. Rok Piltaver, B. Sc.
23. *Maja Somrak, B. Sc., left 01. 09. 14*
24. Aleš Tavčar, B. Sc.
25. Jernej Zupančič, B. Sc.  
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26. Blaž Mahnič, B. Sc.
27. Gašper Pintarič\*, B. Sc.  
Technical and administrative staff
28. Vesna Koricki Špetič, B. Sc.
29. Matej Krebelj
30. Mitja Lasič
31. Liljana Lasič
32. Jure Šorn
33. Lana Zemljak

Note:

\* part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Erik Čuk, Matjaž Gams, Matej Možek, Franc Strle, Vera Maraspin-Čarman, Jurij F. Tasič, "Supervised visual system for recognition of erythema migrans, an early skin manifestation of lyme borreliosis", *Stroj. vestn.*, vol. 60, no. 2, pp. 115-123, Feb. 2014.
2. Erik Dovgan, Matija Javorski, Tea Tušar, Matjaž Gams, Bogdan Filipič, "Discovering driving strategies with a multiobjective optimization algorithm", *Applied soft computing*, vol. 16, no. 1, pp. 50-62, 2014.
3. Matjaž Gams, "The unexpected hanging paradox from an AI viewpoint", *Informatica (Ljublj.)*, vol. 38, no. 2, pp. 181-185, 2014.
4. Matjaž Gams, Matej Horvat, Matej Ožek, Mitja Luštrek, Anton Gradišek, "Integrating artificial and human intelligence into tablet production process", *AAPS PharmSciTech*, vol. 15, no. 6, pp. 1147-1453, 2014.
5. Hristijan Gjoreski, Matjaž Gams, Mitja Luštrek, "Context-based fall detection and activity recognition using inertial and location sensors", *Journal of ambient intelligence and smart environments*, vol. 6, no. 4, pp. 419-433, 2014.
6. Anton Gradišek, Pedro José Sebastião, Susete Nogueira Fernandes, Tomaž Apih, Maria Helena Figueiredo Godinho, Janez Seliger, "<sup>1</sup>H-<sup>2</sup>H cross-relaxation study in a partially deuterated nematic liquid crystal", *J. phys. chem., B Condens. mater. surf. interfaces biophys.*, vol. 118, no. 20, pp. 5600-5607, 2014.
7. Dayana Hristova, Matej Guid, Ivan Bratko, "Assessing the difficulty of chess tactical problems", *Int. j. adv. intell. syst.*, vol. 7, no. 3/4, pp. 728-738, 2014.
8. Boštjan Kaluža, Božidara Cvetković, Erik Dovgan, Hristijan Gjoreski, Violeta Mirchevska, Matjaž Gams, Mitja Luštrek, "A Multiagent care system to support independent living", *Int. j. artif. intell. tools*, vol. 23, no. 1, pp. 1440001-1-1440001-30, 2014.
9. Violeta Mirchevska, "Classifier generation by combining domain knowledge and machine learning", *Informatica (Ljublj.)*, vol. 38, no. 1, pp. 91-92, 2014.
10. Violeta Mirchevska, Mitja Luštrek, Andraž Bežek, Matjaž Gams, "Discovering strategic behaviour of multi-agent systems in adversary settings", *Comput. inform.*, vol. 33, no. 1, pp. 79-108, 2014.
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12. Miha Mlakar, Tea Tušar, Bogdan Filipič, "Comparing solutions under uncertainty in multiobjective optimization", *Math. probl. eng.*, vol. 2014, 2014, pp. 817964-1-817964-10.
13. Maja Somrak, Mitja Luštrek, Jakob Šušterič, Tomo Krivic, Ana Mlinar, Tilen Travnik, Luka Stepan, Mitja Mavsar, Matjaž Gams, "Tricorder: consumer medical devices for discovering common medical conditions", *Informatica (Ljublj.)*, vol. 38, no. 1, pp. 81-88, 2014.
14. Tea Tušar, Bogdan Filipič, "Visualizing exact and approximated 3D empirical attainment functions", *Math. probl. eng.*, vol. 2014, pp. 569346-1-569346-18, 2014.
15. Vedrana Vidulin, Marko Bohanec, Matjaž Gams, "Combining human analysis and machine data mining to obtain credible data relations", *Inf. sci.*, vol. 288, pp. 254-278, dec. 2014.

16. Domen Zupančič, Božidara Cvetković, "Smart-home energy management in the context of occupants' activity", *Informatica (Ljublj.)*, vol. 38, no. 3, pp. 171-180, 2014.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Jure Brence, Žiga Gosar, Vid Seražin, Jernej Zupančič, Matjaž Gams, "Multiobjective optimisation of water heater scheduling", In: *Intelligentni sistemi: zbornik 17. mednarodne multikonference - IS 2014, 7-8 oktober 2014, Ljubljana, Slovenija: zvezek A: proceedings of the 17th International Multiconference Information Society - IS 2014, October 7th-8th, 2014, Ljubljana, Slovenia: volume A*, Rok Piltaver, ed., Matjaž Gams, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 5-8.
2. Božidara Cvetković, Mitja Luštrek, "Analiza možnosti zaznavanja podobnosti med uporabniki", In: *Intelligentni sistemi: zbornik 17. mednarodne multikonference - IS 2014, 7-8 oktober 2014, Ljubljana, Slovenija: zvezek A: proceedings of the 17th International Multiconference Information Society - IS 2014, October 7th-8th, 2014, Ljubljana, Slovenia: volume A*, Rok Piltaver, ed., Matjaž Gams, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 14-17.
3. Matija Černe, Boštjan Kaluža, Mitja Luštrek, "Analiza nakupov in modeliranje pospeševanja prodaje v spletni trgovini Mercator", In: *Intelligentni sistemi: zbornik 17. mednarodne multikonference - IS 2014, 7-8 oktober 2014, Ljubljana, Slovenija: zvezek A: proceedings of the 17th International Multiconference Information Society - IS 2014, October 7th-8th, 2014, Ljubljana, Slovenia: volume A*, Rok Piltaver, ed., Matjaž Gams, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 9-13.
4. Erik Dovgan, Klemen Gantar, Valentin Koblar, Bogdan Filipič, "Detection of irregularities on automotive semiproducts", In: *Intelligentni sistemi: zbornik 17. mednarodne multikonference - IS 2014, 7-8 oktober 2014, Ljubljana, Slovenija: zvezek A: proceedings of the 17th International Multiconference Information Society - IS 2014, October 7th-8th, 2014, Ljubljana, Slovenia: volume A*, Rok Piltaver, ed., Matjaž Gams, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 22-25.
5. Darja Fišer, Aleš Tavčar, Tomaž Erjavec, "sloWCrowd: a crowdsourcing tool for lexicographic tasks", In: *LREC 2014: proceedings, Ninth International Conference on Language Resources and Evaluation*, May 26-31, 2014, Reykjavik, Iceland, Nicoletta Calzolari, ed., [S. l.], ELRA, 2014, pp. 3471-3475.
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7. Matjaž Gams, "Actual extinctions of animals and humans", In: *Kognitivna znanost: zbornik 17. mednarodne multikonference - IS 2014, 9-10 oktober 2014, [Ljubljana, Slovenija]: zvezek C: proceedings of the 17th International Multiconference Information Society - IS 2014, October 9th-10th, 2014, Ljubljana, Slovenia: volume C*, Urban Kordeš, et al, Ljubljana, Institut Jožef Stefan, 2014, pp. 23-28.
8. Matjaž Gams, "Are humans getting smarter due to AI?", In: *Intelligentni sistemi: zbornik 17. mednarodne multikonference - IS 2014, 7-8 oktober*



- 2014, Ljubljana, Slovenija: zvezek A: proceedings of the 17th International Multiconference Information Society - IS 2014, October 7th-8th, 2014, Ljubljana, Slovenia: volume A, Rok Piltaver, ed., Matjaž Gams, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 30-33.
9. Hristijan Gjoreski, Simon Kozina, Matjaž Gams, Mitja Luštrek, "RAREFall - real-time activity recognition and fall detection system", In: *Percom workshops*, 2014 IEEE International Conference on Pervasive Computing and Communication, 24-28 March, Budapest, Hungary, Danvers, IEEE = Institute of Electrical and Electronics Engineers, 2014, pp. 145-147.
  10. Hristijan Gjoreski, Simon Kozina, Mitja Luštrek, Matjaž Gams, "Recognizing human activities and detecting falls in real-time", In: *Zbornik: 1. del: part 1*, 6. študentska konferenca Mednarodne podiplomske šole Jožefa Stefan = 6th Jožef Stefan International Postgraduate School Students' Conference, 20.-22. 05. 2014, Ljubljana, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2014, pp. 121-130.
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  13. Hristijan Gjoreski, Aleksandra Rashkovska, Simon Kozina, Mitja Luštrek, Matjaž Gams, "Telehealth using ECG sensor and accelerometer", In: *MIPRO 2014: proceedings*, (MIPRO ... (CD-ROM)), MIPRO 2014, 37th International Convention, May 26-30, 2014, Opatija, Croatia, Petar Biljanović, ed., Rijeka, Croatian Society for Information and Communication Technology, Electronics - MIPRO, cop. 2014, pp. 283-287.
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  15. Anton Gradišek, Maja Somrak, Mitja Luštrek, Matjaž Gams, "Qualcomm tricorder XPRIZE: a review", In: *Intelligentni sistemi: zbornik 17. mednarodne multikonference - IS 2014, 7-8 oktober 2014, Ljubljana, Slovenija: zvezek A: proceedings of the 17th International Multiconference Information Society - IS 2014, October 7th-8th, 2014, Ljubljana, Slovenia: volume A*, Rok Piltaver, ed., Matjaž Gams, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 42-45.
  16. Vida Groznik, Aleksander Sadikov, Martin Možina, Jure Žabkar, Dejan Georgiev, Ivan Bratko, "Attribute visualisation for computer-aided diagnosis: a case study", In: *ICHI 2014: proceedings*, 2014 IEEE International Conference on Healthcare Informatics, 15-17 September 2014, Verona, VR, Italy, Los Alamitos (California), Washington, Tokyo, IEEE Computer Society, Conference Publishing Services, 2014, pp. 294-299.
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## PATENT APPLICATION

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## PATENT

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2. Matjaž Gams, Tea Tušar, Darko Zadravec, Matej Horvat, *System and method for continuous control and management of tablet manufacturing process*, SI24243 (A), Urad RS za intelektualno lastnino, 30.5.2014.
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## MENTORING

1. Erik Dovgan, *Multiobjective discovery of driving strategies*: doctoral dissertation, Ljubljana, 2014 (mentor Bogdan Filipič; co-mentor Matjaž Gams).
2. Hristijan Gjoreski, *Context-based reasoning in ambient intelligence*: doctoral dissertation, Ljubljana, 2014 (mentor Matjaž Gams; co-mentor Mitja Luštrek).
3. Tea Tušar, *Visualizing solution sets in multiobjective optimization*: doctoral dissertation, Ljubljana, 2014 (mentor Bogdan Filipič).
4. Erik Čuk, *Intelligent system for recognition of erythema migrans*: doctoral dissertation, Ljubljana, 2014 (mentor Jurij F. Tasič; co-mentor Matjaž Gams).



# DEPARTMENT OF REACTOR ENGINEERING

# R-4

*The Department of Reactor Engineering is involved in basic and applied research in the fields of nuclear engineering and safety. Topics include the modelling of basic thermal-hydrodynamic phenomena, thermal-hydraulic safety analyses of design-basis and severe accidents, structural safety analyses and probabilistic safety assessments. Most research activities are part of international cooperation programs. The research results are incorporated into projects for industry and for the regulatory authorities, as well as in under-graduate and doctoral studies programmes.*

## Modelling of basic thermal-hydrodynamic phenomena

Turbulent heat-transfer simulations in low-Prandtl-number liquids were performed using a Direct Numerical Simulation in various computational domains. It was shown that large-scale turbulent structures, which have a weak footprint in the main velocity field statistics, contribute a non-negligible amount of fluctuations in the thermal field. The research was related to the 7<sup>th</sup> EC FP (7th European Commission Framework Programme) project THINS and might be relevant for next-generation fission reactors that will be cooled with liquid metals.

Flow boiling of the refrigerant R-11 in a vertical annular channel was investigated. We simulated experiments performed at the Birine Nuclear Research Center (Algeria) with the ANSYS CFX13 computer code, using a three-dimensional (3D) two-fluid model of subcooled boiling flow. Simulation results successfully predicted the main experimental tendencies associated with variations of the heat flux and the Reynolds number. A sensitivity analysis of several modelling parameters on the radial distribution of the flow quantities highlighted the importance of the correct description of the boiling boundary layer.

Simulations of turbulent flow in a horizontal fuel bundle, using an open-source code, were focused on the performance of various turbulent models in a rod-bundle flow. The results were verified with the MATIS-H experiment (Measurement and analysis of turbulent mixing in sub-channels - horizontal) performed at the Korea Atomic Energy Research Institute.

Intensive Large Eddy Simulations of multiple-jet impingement cooling were continued. The two main mechanisms that contribute to the enhanced heat transfer were revealed: convective cooling by parallel flow near the impingement point and intense stochastic quenching by large-scale vortical structures.

Research on numerical methods in fluid mechanics was continued as well. In the frame of the 7th EC FP project NURESAFE, new theoretical models for interface capturing and sharpening within two-fluid models of two-phase flow were examined. The methods were used to simulate air-water counter-current flow in a vertical pipe, which is related to so-called flooding. A detailed knowledge of basic physical mechanisms of the flooding phenomenon is of particular interest for safety analyses involving loss-of-coolant accidents (LOCA) in nuclear reactors. Within the same project, we considered methods for the uncertainty assessment of 3D computer codes. We used our own Optimal Statistical Estimator (OSE) method to assess the uncertainty of the simulation of mixing of two turbulent flows.

Basic phenomena that might occur during a hypothetical severe accident in a nuclear power plant were investigated. A vapour explosion is an energetic fuel-coolant interaction phenomenon, which may occur if, during an accident, the hot reactor-core melt comes into contact with the coolant. Vapour explosions are an important nuclear-safety issue as they could jeopardize the primary system and the containment integrity. The influence of the metallic zirconium content in prototypic corium on explosion energetics was analysed using experimental results from the OECD Nuclear Energy Agency SERENA project and from the ZREX facility (Argonne National Laboratory, USA). To explain the observed behaviour, the hydrogen film hypothesis limiting the oxidation during premixing was proposed. A comprehensive study of the oxidation influence on fuel-coolant interaction was performed using the MC3D code (Institut de Radioprotection et de Sûreté Nucléaire, France). Furthermore, vapour explosions in stratified melt-coolant configurations



Head:  
**Prof. Leon Cizelj**

**Heat transfer in low-Prandtl-number liquids was analysed using Direct Numerical Simulation of turbulent flow.**

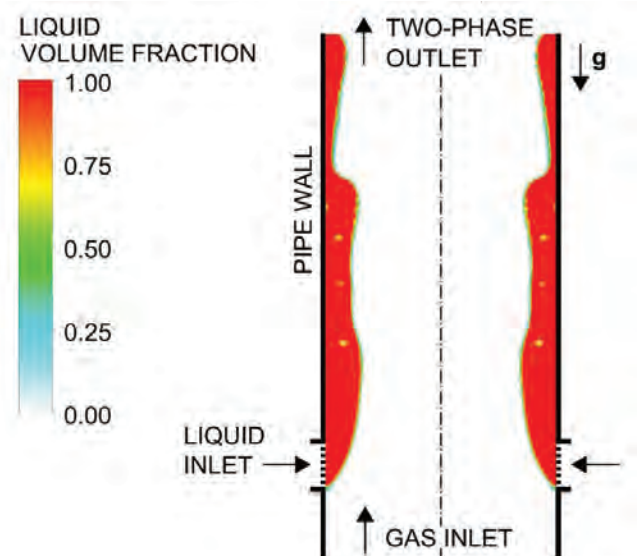


Figure 1: Distribution of liquid volume fraction in simulation of air-water churn flow with accurate interface tracking.



were studied. The recently performed experiments in the PULiMS and SES facilities (Royal Institute of Technology, Sweden) have revealed that strong, stratified explosions may develop spontaneously. A parametric analysis with the MC3D code has shown that the strength of the stratified explosions depends mainly on the premixed melt mass, the melt droplets' size and the water height. Apart from that, the potential of strong vapour explosions during melt-sodium interaction was investigated as well. From the analysis of experiments, a heat-transfer modelling approach for significantly subcooled coolants was proposed. The model was implemented in the MC3D code and the code

**A micromechanical crystal plasticity model was implemented in the computational code ABAQUS to simulate the nonlinear mechanical response of non- and neutron-irradiated stainless steel.**

was used to perform sensitivity simulations in the geometry and with the parameters of the FARO-TERMOS experiments (EC Joint Research Center – JRC – Ispra, Italy). The analyses of the simulation and experimental results indicated that the explosion strength is affected by the melt solidification and the sodium saturated vapour pressure.

In the field of modelling of hydrogen combustion in the containment of a nuclear power plant, we have, in cooperation with Nuclear Research and

Consultancy Group (Netherlands), simulated three experiments on combustion that were performed in the THAI experimental facility (Becker Technologies, Germany). The emphasis was on the testing of different turbulence models, with the purpose to replicate as well as possible the experimental pressure increase and the turbulent flame velocity.

In order to launch our own experimental activities, we are building a laboratory that will be active in the fields of reactor thermal-hydraulics, renewable energy, fluid mechanics and heat transfer on different scales and in different systems. Within the laboratory, an advanced experimental test facility for heat-transfer and fluid-flow studies during single-phase and two-phase flows of pure fluids, mixtures and colloids is being designed and constructed.

**Thermal-hydraulic safety analyses**

Data that are measured in a nuclear plant are of great importance for the assessment of thermal-hydraulic system codes. Namely, the integral effects experimental facilities usually contain atypicalities and scaling distortions relative to full-scale plants. On the other hand, accidents in plants are rare and plant-specific data are generally available only for start-up tests and operational events. A loss of external load in the Krško nuclear power plant, followed by safety systems actuation and reactor trip two minutes later, was analysed with the RELAP5/MOD3.3 best-estimate thermal-hydraulic computer code. In this way, additional information was provided to understand the event. The influence of lead-lag time constants on the signal compensation for safety systems actuation was analysed as well. The results suggest that the RELAP5 code using a standard plant input deck provides an adequate representation of the plant behaviour and could be used for a better understanding of the plant's response when information on all the physical phenomena and processes is not available from measured data.

Within the framework of the European fusion program EUROfusion, a global thermal model of the tokamak for the future fusion reactor DEMO was developed. A conceptual model of the tokamak's geometry was built and complemented by thermal shield systems, structural supports and cryostat. Simulations of the heat transfer are crucial in the design of the tokamak's geometry and of heat removal systems of thermal shields.

An experiment of a small-break LOCA, performed in the TOPFLOW facility (Helmholtz-Zentrum Dresden-Rossendorf, Germany) was simulated with the TRACE computer code. As in many previous investigations of such phenomena, critical flow was found to be the key model for successful theoretical predictions.

We used the system code ASTEC to simulate 9 experiments of hydrogen combustion in a homogeneous atmosphere with upward flame propagation, performed in the THAI experimental facility. Although system codes use a volume-averaged description of the containment, they are suitable for the safety analyses of real plants.

A calculation procedure for the case of a spent-fuel-pit (SFP) accident was upgraded into a method, which, based on monitoring of either the leak rate or dose rate on the edge of the SFP, assesses the pool integrity indirectly in terms of calculating the size and the vertical location of the rupture. This step is essential in the method as it presents the necessary means for predicting

the course of an extreme event, which can be used for assigning the priorities, optimizing absorbed doses and eventually for anticipating the timely evacuation of the site. The above method was further updated so it could be used in the apparatus for assessing the state of a spent-fuel facility. The described method and the apparatus are currently patent pending.

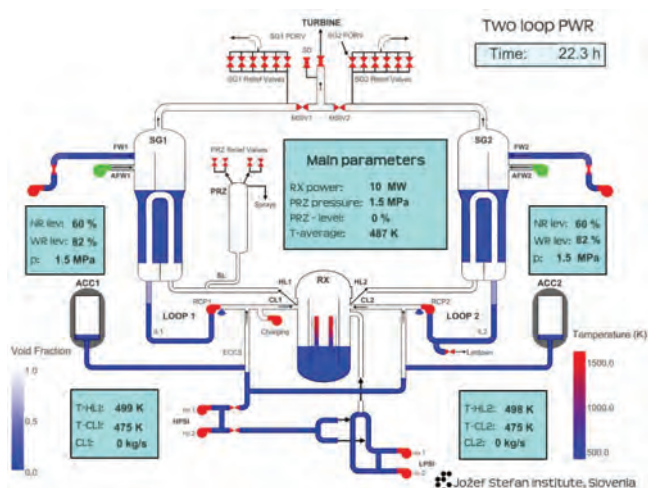


Figure 2: Simulation of transient in Krško nuclear power plant using the RELAP5 code.

### Structural safety analyses

Research remained concentrated on the development of multi-scale computational simulation tools for polycrystalline metallic materials. The focus was set on the improvement of advanced constitutive models for crystal grains and grain boundaries. Data on grains were retrieved either from experimental or analytical methods. The loading of randomly shaped and oriented crystal grains with anisotropic properties resulted in highly inhomogeneous stress fields, which were estimated using the finite-element solver ABAQUS.

Regarding grain-boundary behaviour, a cohesive-zone contact was proposed as an alternative approach to cohesive elements for modelling the intergranular cracking in polycrystalline aggregates. It was established that the numerical convergence issues with the cohesive-zone contact can be significantly smaller compared to the cohesive elements at the same mesh density. The applicability of the approach was demonstrated to both measured (wire) and simulated (Voronoi) microstructures. The work was done in collaboration with the EC JRC in Petten (Netherlands).

In collaboration with the Commissariat à l'Energie Atomique (CEA, France), a micromechanical crystal plasticity model for grains was implemented in ABAQUS to simulate the nonlinear mechanical response of non- and neutron-irradiated 304L austenitic stainless steel. The implementation was validated against CEA results for tensile tests on single-crystal and on simplified polycrystalline models. A local response of the model was evaluated by calculating the normal stress distributions at grain boundaries for wire and Voronoi geometries.

A recently developed approach for the generation of space-continuous and time-dependent temperature fields was employed to reproduce thermal loads in turbulent fluid-mixing conditions of a T-junction case study from the literature. The calculated loads were used to study the 3D structural response of the piping for different boundary conditions. Apart from thermal stresses, the uncertainties in the fatigue life assessment were analysed by means of synthetic temperature signals of different statistics.

We participated in two 7<sup>th</sup> FP EC projects. Within the MULTIMETAL project (structural performance of multi-metal component), finite-element simulations of 2D and 3D homogenous and heterogeneous fracture specimens were successfully performed following various round-robin exercises. Within the FUSION project (plant-level system engineering), thermal expansions and thermal radiation fluxes between the different components of the future fusion reactor DEMO were estimated by numerical simulations. It was found that the thermal expansion is the most critical in the gap between the toroidal field coil magnets and the vacuum vessel.

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**We have developed a new method for optimizing the maintenance activities in a nuclear power plant with consideration of the plant's safety.**

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### Probabilistic safety assessment

A novel method for the optimization of maintenance activities in a nuclear power plant considering the plant safety was developed. The objective function of the optimization is the mean value of the selected risk measure. The optimal solution of the objective function is estimated with a genetic algorithm. The proposed method was applied to a probabilistic safety analysis model of the selected safety system of the reference plant. Results show that the optimization of maintenance could decrease the risk and thus improve the plant safety. The implications of the different constraints in the maintenance on the obtained results were investigated.

An analysis of the introduction of probability distributions associated with component unavailability parameters on the overall unavailability of safety systems of a nuclear power plant was performed. The distribution of the top-event unavailability was assessed using Monte Carlo sampling. The results show that the probability density function of the top event depends on the characteristics of the basic events unavailability distribution and the importance of the selected events. Traditional decision making based on the mean value of the top event unavailability can result in risk underestimation.

A new, dynamic method for a probabilistic assessment of the generation unavailability was developed. The method considers the unavailability implications of the generating unit states, being committed or de-committed as well as their start-up characteristics. The total operating cost of the generating capacities and generating capacities' unavailability were considered. An improved hybrid genetic algorithm was applied to solve the problem. The obtained results indicate the needs and benefits of a more detailed modelling of the power generation availability.

Part of the work was related to international projects. Within the 7th EC FP project ASAMPSA\_E, the state of art in the external hazards screening and multiunit probabilistic safety assessment was analysed and summarized.

### Technical cooperation, consulting services and education

Reactor Engineering Department researchers also cooperated in projects for industry. As an authorized institution for radiation and nuclear safety, we prepared a revised report with proposals for safety improvements of the Krško NPP, based on inspection activities on safety structures, systems and components during the plant's 2013 outage. The revised report considers start-up tests at nominal power that were performed afterwards.

For the utility company GEN energy, we delivered a 7-day course on nuclear reactor thermal-hydraulics. The course covered thermodynamics, fluid mechanics, heat transfer, system codes for thermal-hydraulic analyses, basics of reactor physics and numerical methods.

Members of the department are also actively involved in nuclear engineering under-graduate, master and doctoral studies at the Faculty of Mathematics and Physics at the University of Ljubljana. The programmes are associated with the European Nuclear Education Network (ENEN).

### Some outstanding publications in the past year

1. Tiselj, I.: Tracking of large-scale structures in turbulent channel with direct numerical simulation of low Prandtl number passive scalar, *Physics of Fluids*, 26 (2014), 125111-1-125111-17
2. Draksler, M., Ničeno, B., Končar, B., Cizelj, L.: Large eddy simulation of multiple impinging jets in hexagonal configuration - Mean flow characteristics, *International Journal of Heat and Fluid Flow*, 46 (2014), 147-157
3. Costa Garrido, O., El Shawish, S., Cizelj, L.: A novel approach to generate random surface thermal loads in piping, *Nuclear Engineering and Design*, 273 (2014), 98-109
4. Volkanovski, A., Cizelj, L.: Nuclear power plant maintenance optimization with heuristic algorithm, *Science and Technology of Nuclear Installations*, 2014 (2014), 458016-1-458016-13

### Organization of conferences, congresses and meetings

1. CESAM 1st Periodic Workshop and 1st Steering Committee Meeting: JSI - Reactor Centre, Ljubljana, Slovenia, 18-21 March 2014
2. Course "Nuclear thermal hydraulics": GEN energija d.o.o., Krško, Slovenia, 9-17 June 2014
3. Meeting of NEWHAM project partners: JSI - Reactor Centre, Ljubljana, Slovenia, 26-27 June 2014

## INTERNATIONAL PROJECTS

1. 7FP - EURATOM - ENEN-III; European Nuclear Education Network Training Schemes  
Prof. Leon Cizelj  
European Commission
2. 7FP - EURATOM - TRANSAFE; Training Scheme on Nuclear Safety Culture  
Dr. Andrej Prošek  
European Commission
3. 7FP - EURATOM - THINS; Thermal-hydraulics of Innovative Nuclear Systems  
Prof. Iztok Tiselj  
European Commission
4. 7FP - EURATOM; MULTIMETAL; Structural Performance of Multi-metal Component  
Prof. Leon Cizelj  
European Commission
5. 7FP - NURESAFE; Nuclear Reactor Safety Simulation Platform  
Dr. Boštjan Končar  
European Commission
6. 7FP - CESAM; Code for European Severe Accident Management  
Asst. Prof. Ivo Kljenak  
European Commission
7. 7FP - ASAMPESA\_E; Advanced Safety Assessment: Extended PSA  
Dr. Andrija Volkanovski  
European Commission
8. 7FP - ARCADIA; Assessment of Regional Capabilities for New Reactors Development through an Integrated Approach  
Prof. Leon Cizelj  
European Commission
9. Training and Tutoring for Experts of the NRAs and their TSOs for Developing and Strengthening their Regulatory and Technical Capabilities - INSC Project MC.03/10-LOT 1: Training and Tutoring for Nuclear Regulatory Authorities and their TSO's  
Prof. Leon Cizelj  
ITER-consult SRL
10. Better Understanding and Recognition of Nuclear Skills and Qualifications  
Prof. Leon Cizelj  
University Politehnica of Bucharest
11. Comprehensive and Reliable Prediction of LWR's Internals Mechanical Behavior based on Microstructure-informed Modeling  
Dr. Samir El Shawish  
Slovenian Research Agency
12. Influence of Oxidation and Large Solidification Temperature Range of Fuel Coolant Interaction  
Dr. Matjaž Leskovar  
Slovenian Research Agency
13. SNETP General Assembly; Meeting of the Management Board SNETP

- Prof. Leon Cizelj  
Slovenian Research Agency
14. RU-FU, EUROFUSION; Research Unit - Administration and Services  
Dr. Boštjan Končar  
European Commission
  15. Education-ED-FU, EUROFUSION  
Dr. Boštjan Končar  
European Commission
  16. Plant Level System Engineering-PMI-PPPT-FU, EUROFUSION  
Dr. Boštjan Končar  
European Commission

## RESEARCH PROGRAM

1. Reactor Engineering  
Prof. Leon Cizelj

## R & D GRANTS AND CONTRACTS

1. Experiment and Simulation of Hydrogen Combustion in Nuclear Power Plant Containment Experimental Facility  
Prof. Borut Mavko
2. Development of Methods and Models for Simulation of Thermal-hydraulic Phenomena in Innovative Nuclear Reactors  
Prof. Iztok Tiselj
3. Steam explosions in sodium cooled fast reactors  
Dr. Mitja Uršič

## NEW CONTRACTS

1. Cooperation in an International CAMP Program  
Dr. Andrej Prošek  
Krško Nuclear Power Plant
2. Expert Assessment of Outage, Procedures and Tests during the Shutdown of Krško NPP  
Ljubo Fabjan, M. Sc.  
Milan Vidmar Electrotechnical Institute
3. Course "Nuclear Thermalhydraulics"  
Prof. Leon Cizelj  
ZEL-EN, d. o. o.
4. Course "Nuclear Thermalhydraulics"

Prof. Iztok Tiselj  
Gen energija, d. o. o.

5. The role of Brestanica Thermal Power Plant in Ensuring Krško Nuclear Power Plant Safety

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1. Dr. Michael Buck: Universität Stuttgart, Institut für Kernenergetik und Energiesysteme, Stuttgart, Germany, 18-21 March 2014
2. Dr. Jean-Pierre Van Dorsselaere: Institut de Radioprotection et de Sûreté Nucléaire, Fontenay-aux-Roses, France, 18-21 March 2014
3. Dr. Mykola Džubinský: European Commission, Brussels, Belgium, 18-21 March 2014
4. Dr. Alexandre Ezzidi: AREVA, Courbevoie, France, 18-21 March 2014
5. Dr. Luis E. Herranz: Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas, Madrid, Spain, 18-21 March 2014
6. Prof. Marco Koch: Ruhr-Universität Bochum, Bochum, Germany, 18-21 March 2014
7. Dr. Pal Kostka: NUBIKI Nuclear Safety Research Institute, Budapest, Hungary, 18-21 March 2014
8. Dr. Ghislain Pascal: Institute for Energy and Transport, EC Joint Research Center, Petten, Netherlands, 18-21 March 2014
9. Dr. Felice De Rosa: Italian Nat. Agency for New Technologies, Energy and Sustainable Economic Dev., Rome, Italy, 18-21 March 2014
10. Dr. Victor Sanchez: Karlsruhe Institute of Technology, Karlsruhe, Germany, 18-21 March 2014
11. Dr. Martin Sonnenkalb: Gesellschaft für Anlagen - und Reaktorsicherheit, Köln, Germany, 18-21 March 2014
12. Dr. Virginijus Vileiniškis: Lithuanian Energy Institute, Kaunas, Lithuania, 18-21 March 2014
13. Dr. Henrique Austregesilo: Gesellschaft für Anlagen - und Reaktorsicherheit, Köln, Germany, 26-27 June 2014
14. Mr. Frederic Daude: Electricité de France, Clamart, France, 26-27 June 2014
15. Mr. Pascal Galon: Commissariat à l'Energie Atomique, Gif-sur-Yvette, France, 26-27 June 2014
16. Dr. Attila Imre: MTA-EK Centre for Energy Research, Hungarian Academy of Sciences, Budapest, Hungary, 26-27 June 2014
17. Dr. Ed Komen: NRG Nuclear Research and Consultancy Group, Petten, Netherlands, 26-27 June 2014
18. Dr. Pavel Kral: ÚJV Řež, Husinec, Czech Republic, 26-27 June 2014
19. Mr. Dirk Lucas: Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany, 26-27 June 2014
20. Dr. Bojan Ničeno: Paul Scherrer Institut, Villigen, Switzerland, 26-27 June 2014
21. Dr. Jean-Marie Seynhaeve: Université Catholique de Louvain, Louvain-la-Neuve, Belgium, 26-27 June 2014
22. Dr. Arris Tijsseling: Technische Universiteit Eindhoven, Eindhoven, Netherlands, 26-27 June 2014
23. Dr. Mindaugas Vainoras: Lithuanian Energy Institute, Kaunas, Lithuania, 26-27 June 2014
24. Prof. Igor Piore: University of Ontario Institute of Technology, Ontario, Canada, 22-24 October 2014
25. Ms. Natalia Kozioura: Journal of Nuclear Engineering and Radiation Science, Ontario, Canada, 22-24 October 2014
26. Dr. Renaud Meignen: Institut de Radioprotection et de Sûreté Nucléaire, Fontenay-aux-Roses, France, 5-6 November 2014
27. Dr. Stephane Picchi: Institut de Radioprotection et de Sûreté Nucléaire, Fontenay-aux-Roses, France, 5-6 November 2014

*Participants of NEWHAM meeting (14), among them:*

13. Dr. Henrique Austregesilo: Gesellschaft für Anlagen - und Reaktorsicherheit, Köln, Germany, 26-27 June 2014

## STAFF

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6. Dr. Matjaž Leskovar
7. Asst. Prof. Marko Matkovič
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12. Dr. Blaže Gjorgiev, left 01. 06. 14
13. Dr. Duško Kančev, left 01. 02. 14
14. Dr. Mihaela - Irina Uplaznik, left 01. 04. 14

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15. Ovidiu-Adrian Berar, B. Sc.
16. Raphael Stephane Connes, B. Sc., left 01. 05. 14
17. Oriol Costa Garrido, B. Sc.
18. Martin Draksler, B. Sc.
19. Romain Claude Francis Henry, B. Sc.
20. Tadej Holler, B. Sc.
21. Blaž Mikuž, B. Sc.
22. Jure Oder, B. Sc.
23. Matej Tekavčič, B. Sc.
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26. Tanja Klopčič
27. Urška Knific Terze, B. Sc.
28. Zoran Petrič, B. Sc.

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Boštjan Končar, Martin Draksler, "Divertor high flux helium cooling: large eddy simulation (LES) of multiple jet impingement case", In: *Final report 2007-2013 of the Association EURATOM-MESCS*, Boštjan Končar, ed., Bojan Žefran, ed., Ljubljana, Slovenska fuzijska asociacija, 2014, pp. 115-120.
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4. Matjaž Leskovar, Boštjan Končar, Igor Lengar, Samo Košmrlj, "Assesment of interface between MCNP and ANSYS CFX for the blanket test case", In: *Final report 2007-2013 of the Association EURATOM-MESCS*, Boštjan Končar, ed., Bojan Žefran, ed., Ljubljana, Slovenska fuzijska asociacija, 2014, pp. 103-110.

## PROFESSIONAL MONOGRAPH

1. Ovidiu-Adrian Berar, Andrej Prošek, *Assessment against ACHILLES reflood experiment with TRACE V5.0 Patch3*, (International agreement report, NUREG/IA-0441), Washington, U. S. Nuclear Regulatory Commission, 2014.

## PATENT APPLICATION

1. Marko Matkovič, Iztok Tiselj, Ivo Kljenak, Andrej Prošek, Matjaž Leskovar, Ljubo Fabjan, Leon Cizelj, *Method and apparatus for assessing the state of a spent-fuel facility*, GB1409900.6, Intellectual Property Office, 4.6.2014.



# REACTOR INFRASTRUCTURE CENTRE

# RIC

***The Reactor Infrastructure Centre (RIC) incorporates a research reactor, the 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.***



Head:  
**Prof. Borut Smodiš**

Besides operating and maintaining the reactor, the members of the reactor staff participate in other activities requiring specialists skilled in the work with sources of radiation and in reactor technology, such as the servicing of industrial radioactive sources and the surveillance of the fuel management at NPP Krško.

The reactor is operated in accordance with a program approved by the RIC and the Radiation Protection Unit - RPU (SVPIS in Slovenian language) for each week. In 2014 the reactor operated for 142 days and produced 96.7 MWh of heat. Altogether, 579 samples were irradiated in the rotary specimen rack and 48 in the pneumatic transfer system. Neutron-activation analyses with approximately 400 samples was made for the Department of Environmental Sciences O2, and the reactor operated for approximately 200 hours.

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.

In 2014 the reactor was mainly used as a neutron source for neutron-activation analysis, the irradiation of electronic components and education. For educational purposes it was mostly used for the needs of the J. Stefan Institute's Nuclear Training Centre. For the irradiation of samples it was mostly used by the Department of Environmental Sciences O2 and the Department of Experimental Particle Physics F9. The Reactor Physics Department F8 used the reactor for experiments of reactor physics, and the Reactor Engineering Department R4 used the reactor for thermal-hydraulic experiments.

In the Hot Cells Facility the activities were mostly performed by the Department of Environmental Sciences O2, the Radiation Protection Unit and the Slovenian Agency for Radioactive waste Management (ARAO) - processing and preparation of radioactive waste for storage needs.

The reactor was used for the following research:

- Reactor physics and neutronics
- Activation analysis
- Research on radiation damage to semiconductors
- Neutron dosimetry and spectrometry
- Neutron radiography
- Activation of materials, nuclear waste and decommissioning
- Irradiation of materials for fusion reactors
- Irradiation of electronic and medical components
- Development and testing of new detectors
- Development of new methods for measuring power profiles, neutron spectra, etc.
- Verification and validation of methods for calculating the transport of neutrons, photons and electrons
- Development of educational tools in reactor physics.

Since 2011, The TRIGA reactor has participated in the FP7 AIDA (Advanced Infrastructures for Detectors and Accelerators) project that brings together advanced European infrastructures for future particle-physics experiments. The AIDA project was completed at the end of 2014. In 2015, it started a new project, "AIDA 2".

Within the frame of the "Experimental Verification of Kinetic Parameters of the TRIGA Reactor and the Upgrade of the Digital Meter of Reactivity" some experiments were conducted. For these purposes the reactor operated for about 20 hours.

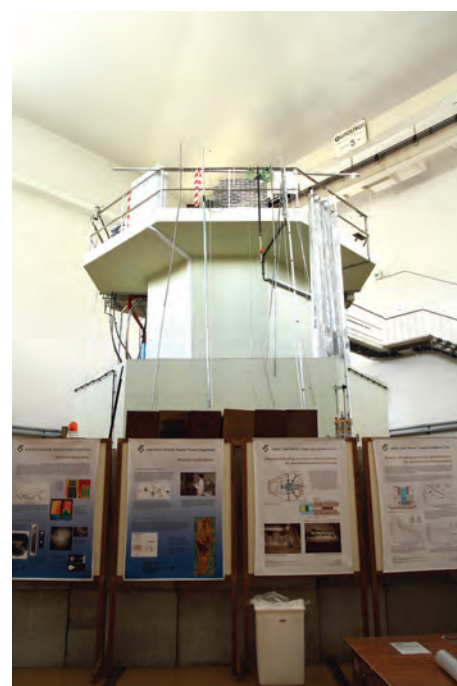


Figure 1: TRIGA Reactor





Figure 2: Reactor core

Within the international collaboration with the CEA, France, we tested the resistance of polyethylene capsules to thermal neutrons (project Design of an irradiation device for FT-TIMS method at the JSI TRIGA Mark II reactor) and performed preliminary measurements of the fission and ionisation chambers' response (project name: Experimental verification of the flux from factors and qualification of wide range neutron instrumentation).

In collaboration with the reactor physics division and CEA France a series of experiments were performed in order to determine the kinetic parameters of the reactor. This was the first time the measurements were performed with four fission chambers simultaneously. In addition, the new CEA-developed system, called SPECTRON, was tested. Within the framework of this project the control rod worth measurement methods were improved. In another CEA project the IRDF dosimetry library was tested by the reactor physics division and the CEA. The calculations were compared with activation measurements at the TRIGA reactor in order to accurately determine the neutron spectra in the irradiation channels.

In order to investigate the possible use of the  $^{55}\text{Mn}(n,\gamma)^{56}\text{Mn}$  reaction as a T monitor in fusion reactors, we irradiated reference materials (Al-1%Mn and Al-0.1%Au, TLD(LiF) and LiPb) in the reactor irradiation channels. The reactor operated during approximately 10 hours for this purpose.

The projects within the framework of IAEA Technical Coordination Programme entitled "Carrying out a Feasibility Study and Installing the Thermal Neutron Driven 14 MeV Neutron Converter into the TRIGA Research Reactor" and "Installation of DT converter of neutrons in the TRIGA reactor" was continued.

Before the reactor start-up at NPP Krško, preparations and tests to conduct physical tests took place at the TRIGA reactor.

The project "Irradiation and Analysis for Si samples", with its start in 2013, within the framework of the contract with Institute of Radiation Problems of AzNAS, Azerbaijan, was continued also in 2014. Various samples were irradiated in the TRIGA reactor and analysed in cooperation with some JSI departments.

The work on Periodic Safety Report that started in 2011, continued. The project was completed at the end of 2014.

In November 2012 an IAEA INSARR mission was conducted. The objectives of the mission was to review the operational safety of the reactor, including reactor management and regulatory supervision, Safety Analysis Report, safety analyses, Operational Limits and Conditions, conduct of operations, maintenance, training and qualifications of the operating personnel, utilization and modifications, operational radiation protection and waste management, emergency planning, quality assurance and decommissioning plan. The work on recommended issues was carried out in 2013 and was continued in 2014.

Practical exercises in reactor physics and kinetics for the students of physics at the University of Ljubljana were performed. The postgraduate students of nuclear engineering attended some of these exercises as well. For these purposes the reactor operated for approximately 3 months, and the average number of participants in the exercise were 12. The reactor was also used for practical exercises within the training program of the NPP Krško reactor operators (practical training in the area of secure and efficient operation of nuclear reactors), lasting from 6 October 2014 to 3 March 2015, and which was attended by 21 participants.

All 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 2014, there were more than 50 short group visits to the reactor. The visitors were mainly foreign scientists, students and 30 groups of school children. Their total number was more than 1500.

The research results were published in approximately 20 scientific papers. Five young researchers performed their research at the reactor.

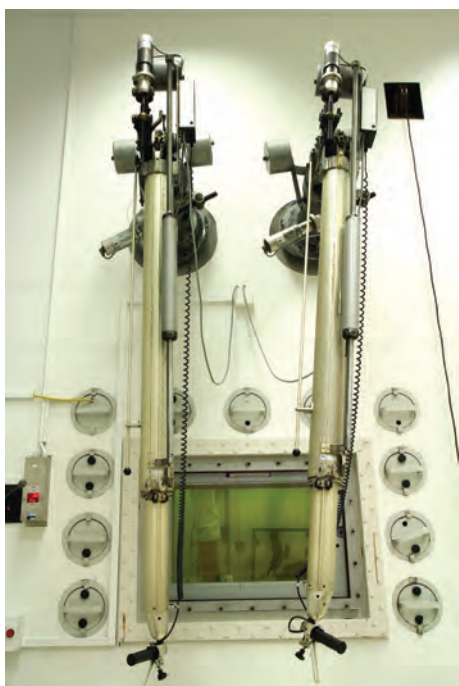


Figure 3: Hot cell

## INTERNATIONAL PROJECTS

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. Irradiations in TRIGA Nuclear Reactor<br/>Prof. Borut Smodiš<br/>European Organization for Nuclear Research</li> <li>2. Training in Radiochemistry and Radioactivity Measurements for Practitioners from Countries Eligible under the JRC Enlargement &amp; Integration Policy<br/>Prof. Borut Smodiš<br/>Institute for Reference Materials and Measurements</li> <li>3. Feasibility Study and Installation of Thermal Neutron Driven 14 MeV Neutron Converter</li> </ol> | <ol style="list-style-type: none"> <li>into the TRIGA Research Reactor<br/>Asst. Prof. Luka Snoj<br/>IAEA - International Atomic Energy Agency</li> <li>4. Automation of a Pneumatic Transport System for Neutron Activation Analysis<br/>Prof. Borut Smodiš<br/>IAEA - International Atomic Energy Agency</li> <li>5. NATO SPS.EAP.SFP 984524: Radioactive and Heavy Metal Waste Tailings - Risk Reduction in Fergama Valley, Kyrgyz Republic</li> </ol> |
|---|---|

Prof. Peter Stegnar

NATO - North Atlantic Treaty Organisation

6. IAEA Fellowship for Mr Alain Kalala Tshiamu (ZAI/13011)  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency
7. IAEA Fellowship for Mr Bashar Salim Al-Jaafreh (JOR/13033)  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency
8. IAEA Fellowship for Mr Ismail Marrhich (MOR/13012), 1 September-30 November 2014  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency
9. IAEA Fellowship for Mr Said Otmani (MOR/13013), 1 September-30 November 2014  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency
10. IAEA Fellowship for Mr Hassane Graine (C6/ALG/11007), 1 September-30 September 2014  
Prof. Borut Smodiš  
IAEA - International Atomic Energy Agency

## R & D GRANTS AND CONTRACTS

1. Irradiation and Analysis of Si Samples  
Anže Jazbec, B. Sc.
2. Irradiation for FT-TIMS Method at the JSI TRIGA Mark II Reactor  
Asst. Prof. Luka Snoj
3. Irradiation and Analysis of Nano Si Samples  
Anže Jazbec, B. Sc.

## NEW CONTRACT

1. Treatment and Conditioning of Radioactive Waste for Storage in Hot Cells Facility  
Prof. Borut Smodiš  
ARAO

## VISITORS FROM ABROAD

1. Alain Kalala Tshiamu, Commissariat General a l'Energie Atomique, Campus Universitaire de Kinshasa, Kinshasa XI, Republique democratique du Congo, 17.03.2014 - 02.05.2014
2. Bashar Salim Al-Jaafreh, Nuclear Safety and Security Directorate, Jordan Nuclear Regulatory Commission, Amman, Jordan, 24.03.2014 - 24.06.2014
3. Hassane Graine, Centre de Recherche Nucleaire de Birine, Commissariat a l'energie atomique, Djelfa, Algeria, 30.08.2014 - 01.10.2014
4. Ismail Marrhich, Centre national de l'energie, des sciences et des techniques nucleaires, CNSTEN - Rabat, Rabat, Morocco, 30.08.2014 - 28.11.2014
5. Said Otmani / Centre national de l'energie, des sciences et des techniques nucleaires, CNSTEN - Rabat, Rabat, Morocco, 30.08.2014 - 28.11.2014
6. Niklas Barringer, ISEC Industrial Security AB, Höganäs, Sweden, 12.09.2014

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### Technical officer

3. Dr. Tinkara Bučar

### Technical and administrative staff

4. Andrej Gyergyek, B. Sc.
5. Darko Kavšek, B. Sc.
6. Marko Rosman
7. Sebastjan Rupnik, B. Sc.

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3. Borut Smodiš, Marko Štrok, Marko Černe, "Radioecology around a closed uranium mine", *J. radioanal. nucl. chem.*, vol. 299, issue 1, pp. 765-771, 2014.

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2. Ivan Aleksander Kodeli, Vladimir Radulović, Darko Kavšek, W. Pohorecki, T. Kuc, "TRIGA irradiations of Mn foils and TLD as potential Tritium production monitors for fusion applications", In: *Proceedings, 23rd International Conference Nuclear Energy for New Europe - NENE 2014, Portorož, Slovenia, September 8-11, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2014, 9 pp.*
3. Luka Snoj, Sebastijan Rupnik, Anže Jazbec, "Advanced reactor physics exercises at the TRIGA Mark II reactor", In: *Transactions: RRFM*

*European Reactor Conference 2014, Ljubljana, Slovenia, 30 March - 3 April 2014*, (ENS conference), Brussels, European Nuclear Society, 2014, 9 pp.

4. Luka Snoj, Sebastijan Rupnik, Anže Jazbec, "New practical exercises at the JSI TRIGA Mark II reactor", In: *PHYSOR 2014 International conference, PHYSOR 2014 International Conference, The role of reactor physics towards a sustainable future*, Sep.28-Oct.3, 2014, Kyoto, Kyoto, PHYSOR, 2014, 12 pp.
5. Luka Snoj, Sebastijan Rupnik, Anže Jazbec, "New training experiments at the JSI TRIGA Mark II reactor", In: *Proceedings, 23rd International Conference Nuclear Energy for New Europe - NENE 2014, Portorož, Slovenia, September 8-11, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2014, 10 pp.*
6. Luka Snoj, Andrej Trkov, Igor Lengar, Anže Jazbec, Vladimir Radulović, Gašper Žerovnik, P. Sauvan, F. Ogando, Jesús Sanz, "Feasibility study of installing a thermal 14 MeV neutron converter into a research nuclear reactor", In: *PHYSOR 2014 International conference, PHYSOR 2014 International Conference, The role of reactor physics towards a sustainable future*, Sep.28-Oct.3, 2014, Kyoto, Kyoto, PHYSOR, 2014, 14 pp.
7. Gašper Žerovnik, Tanja Kaiba, Vladimir Radulović, Anže Jazbec, Sebastijan Rupnik, L. Barbot, D. Fourmentel, Luka Snoj, Jean-François Villard, "Validation of the neutron and gamma flux distributions in the JSI TRIGA reactor core", In: *Proceedings, 23rd International Conference Nuclear Energy for New Europe - NENE 2014, Portorož, Slovenia, September 8-11, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2014, 9 pp.*

## MENTORING

1. Marko Černe, *Transfer of natural radionuclides to selected organisms from soil contaminated with U-mill tailings*: doctoral dissertation, Ljubljana, 2014 (mentor Borut Smodiš).
2. Bolat M. Uralbekov, *Isotopic signatures of U series radionuclides in the natural water environment of Central Asian uranium sites*: doctoral dissertation, Ljubljana, 2014 (mentor Peter Stegnar; co-mentors Mukhambetkali Burkitbayev, Borut Smodiš).

# NETWORKING INFRASTRUCTURE CENTRE

# NIC

**The Networking Infrastructure Centre (NIC) is responsible for the administration, development, management and expansion of the core network and ICT services and infrastructure for the Jožef Stefan Institute. It also provides the development of computing, communication, data and security infrastructure for the research departments, centres and services of the institute.**

The NIC's main mission is to provide a high level of connectivity and integration to the local and international communication networks and infrastructures for research departments, programmes, groups and projects and to provide ICT support for the research activities at the Jožef Stefan Institute, including the development, management and administration of the ICT and computing infrastructure, technology, facilities and services at the institute. We work in four main domains: networking infrastructure, network security, network services and distributed network computing.

## Networking infrastructure

The Networking Infrastructure Centre provides development, management, administration and support to the physical networking infrastructure for the JSI and support to local networks so as to enable internal and internet connectivity to the users and services at the JSI. This task includes the management of wireless networks at the JSI's locations and a number of dedicated networks for specific services, projects and activities (i.e., dedicated links to other institutions, secure links to the Reactor Infrastructure Centre Podgorica, etc.).

*Physical network:* In accordance with development of the JSI and the increased requirements of several research groups and organizational units, we have continued the on-going extension and optimisation of the physical network in the past year. A number of core backbone routing and switching upgrades enabled us to optimize for higher throughput and lower latency as well as expanding the network and its support for virtual network links and the IPv6 protocol.

In the course of ongoing physical network infrastructure upgrades at the Reactor Infrastructure Centre Podgorica campus, where the existing physical link of the campus was upgraded to 10 Gbit/s capacity in 2013, we continued to upgrade the internal network and active components to support the managed VLAN and the integration of the RIC network with the core network, while enhancing support for secure remote VLAN access to the campus network in addition to the JSI's VPN.

Existing external 10 Gbit/s connection via the ARNES and GÉANT networks with the dedicated LHCONe network (LHC Open Network Environment) used for high network throughput for the ATLAS project inside the WLCG (Worldwide Large Hadron Collider Computing Grid) and the distributed Nordic computing T1 cloud has been replaced in order to use GÉANT's Multi-Domain VPN and allow operations at lower technical and financial cost for the ARNES and Nordic NREN networks. The implemented redistribution between the relevant OSPF area and the BGP, used on the LHCONe network, enabled us to easily make changes and deploy potential additional MDVPN or dedicated international connections (also known as light-paths).

*Monitoring:* In addition to existing traffic, event and status-monitoring infrastructure based on the software packages Nagios, Ganglia, Cacati and Observium, we have introduced a new, flexible, analytical facility to improve our dynamic response to changes in usage and traffic and to the detection of exceptional events in the context of the JSI's network. The new system is built around the analytical visualisation package Kibana with Elasticsearch as a backend. The package is connected to an internally developed stack of filters and aggregators to enable us to react to usage and events in the domains of web services, security policies, firewalls, authentication and authorization, network time systems, e-mail delivery, analysis, processing and security systems, etc. In addition, we have extended the system for environmental monitoring that was developed in-house and deployed in 2013 with additional sensors



Head:  
**Vladimir Alkalaj, M. Sc. \***

**Modern, up-to-date 10 Gbit/s network backbone, IPv6 protocol and dedicated external links is the basis of a flexible modern network at the Jožef Stefan Institute that has to support high availability and advanced services with many fixed and wireless clients.**

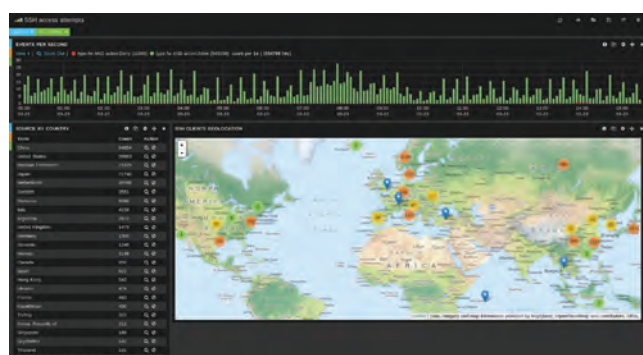


Figure 1: Modern monitoring, visualisation and analysis tools: Kibana showing the temporal and spatial distribution of ssh connections, including ssh password cracking attempts.

\*Photo by Sašo Radelj



and denser deployment. The system allows us to deploy higher-density racks in the computing centre, while minimising any equipment damage due to overheating. Our in-house firmware and driver solution ensures integration with standard protocols (SNMP) and interoperability with existing monitoring systems. The upgrade of the cooling

**Internal development of e-mail security and dynamic network firewalling, virtual networks, and advanced analysis and monitoring ensure the security of an open academic network in the age of a hostile Internet.**

system has enabled us to finally provide suitable working conditions in the main data centre again, but future growth is still hampered due to space limitations, and so a new centre is still needed.

*Wireless network:* Because of the increasing use of the wireless network due to new users and due to the fact that users use multiple devices simultaneously, we have to continue with the deployment of new wireless access points in order to improve the coverage and ensure useful signal density at

the critical points. Software-controlled directional shaping of the radio coverage has improved the efficiency of the existing resources.

*IPv6 support:* Continuous upgrading and improvements in the network-router protocol stack provides flexible support for new protocols. Support for the IPv6 protocol stack across all the network segment is crucial as part of our long-term strategy to alleviate the load on the already mostly spent IPv4 address pool. As an example, RADIUS authentication over the IPv6 stack is now supported.

**Network security**

The NIC is responsible for implementing security measures and policies in three domains: external network connectivity security, security of the network itself and security of the services and software deployments. External network security is provided by the dynamic management and configuration of an active deep-packet inspection firewall system and routing configuration, with the exception of dedicated links where passive measures (configuration, filtering and supervision) are used. Constant dynamic supervision, traffic monitoring and event analysis is necessary to ensure suitable security in the complex constraints and requirements of an open academic network that collide with current security considerations due to the increased detection of threats from the outside network. Therefore, ensuring a secure and open environment requires disproportionate increases in equipment capabilities and efforts in the dynamic security policy configuration. In 2014, we have alleviated the situation with upgrades and extensions to the monitoring and logging infrastructure, including those covering security and web services, and implemented interfaces and filters for an efficient dynamic analysis and visualisation framework based on Kibana and ElasticSearch.

Since the NIC is responsible for the security of the ICT infrastructure of the institute, we are active members of the relevant institutions and groups, notably the national security response centre SICERT, FIRST (Forum of Incident Response and Security Teams), EGI CSIRT (European Grid Initiative distributed computing security incident response team), we are part of the response team of the national distributed computing network SLING (Slovenian Initiative for National grid). The national science certificate agency SiGNET CA (Slovenian Grid Network Certification Authority), managed by the NIC, is a full member of EU Grid PMA (EU Grid Policy Management Authority) and IGTF (Interoperable Global Trust Federation). We have participated in the creation of the Slovenian network technology and security association SINOG (Slovenian Network Operators Group) and the organization of its first events, including the first technical workshop hosted at the JSI.

*E-Mail:* In the field of e-mail security and protection against undesired or malignant messages we have continued with our in-house software development. Support for international encoding using Unicode UTF-8 has been improved, notably in the SpamAssassin package, where changes have become part of the free software release. SMTPUTF-8 has been included in Postfix, which brings protocol-level improvements to UTF-8 support in the stack. In addition and in support of these changes, the international domain name handling in our DNS implementation has been improved.

*Cryptography and certification:* We have continued with gradual DNSSEC signed internet domain integration using automated mechanisms for the verification of signatures and with the preparation for the gradual introduction of the DANE system (integration of TLS certificates with the DNS system) in e-mail transfers and publishing SSHFP records via DNS servers. The number of issued digital certificates based on the SiGNET CA scientific certificate PKI system has increased, but also many free COMODO server certificates, courtesy of Arnes support, have been issued for services that are offered to the general public, since COMODO certificates are recognised by the major operating systems and browsers. We have enlarged the use of the VPN infrastructure, intended to enable users at remote locations to connect to the JSI's network securely, and added support for VPN connections to the user network at the Reactor Infrastructure Centre Podgorica. The system is mostly used by researchers at foreign conferences and exchanges, users who have

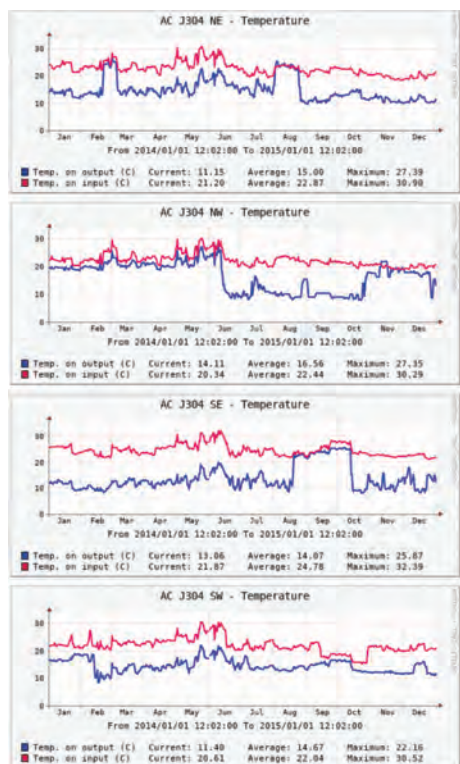


Figure 2: Cacti, a standard tool, displaying temperature fluctuation as measured by one of the sensors in the data centre.

to deal with foreign networks that block certain types of connections, and users working from home. The VPN is quite resilient and capable of transferring data over a virtual HTTPS-embedded connection, circumventing such measures, and also enables remote users to access services such as subscription-based scientific journals.

### ICT services

The NIC provisions, develops and maintains a number of core and secondary core ICT services. The most important among these are e-mail (e-mail routing and delivery, in-box management, directory management, webmail services etc.) and World Wide Web support (central web server, web hosting for users, departments and projects, web directory). Secondary ICT services are provided in support of certain core or specific activities at the JSI, such as web presentations, a conference system, supervision and monitoring, etc. In some of these services the NIC is directly invested in the software or infrastructure development, such as the network time services and e-mail filtering and security, while others are simply administered and maintained. The third NIC service category is comprised of services supporting our users (calendar, event management, directories) and software/system developers (code repositories, integration and verification, licence management, mobile platform software development, integration and shipping for Apple Appstore, Blackberry World, Google Play and Microsoft Store). In addition, we provide physical server hosting and management, aimed primarily at larger projects and systems, the administration of directories for personal computing and user management (such as departmental single sign-on or directory services) and the administration of mission-critical workstations and components.

In 2014 we continued the work on improving our systems automation and provisioning to manage the increasing load on our personnel due to higher demands and the increase in user numbers, network traffic and supported services. The upgrade of the cooling systems has permitted us to create an acceptable environment for the stable functioning of existing services, but for further additions to installed equipment the current data centre is inadequate, due to size and electricity limitations, which has postponed a number of larger projects (new archival systems, off-site backup system arrangement with Reactor Infrastructure Centre Podgorica, on-demand physical and virtual servers and data servers for temporary data storage) to the end of 2015, after the planned addition of a new data-centre room.

We have expanded our web-hosting activity (over 65 distinct virtual servers) and completely re-engineered the core JSI web server to make it more robust and better integrated with the Kibana analysis and visualization system. This has enabled us to streamline the implementation, resolve a number of security and optimization issues and prevent the servicing of unwanted requests. The increased load on our personnel due to the demands for hosting and services is forcing us to continue our automated provisioning efforts which are planned to culminate in fully automated virtual and physical services on demand.

We have continued the updating of our user-facing documentation and our user interfaces. A Single-Sign-On (SSO) service, integrated with the national AAI federation at Arnes and European eduGAIN federation has been introduced, and thus our users can now access numerous national and international services using their institute credentials. At the same time, the new feature is meant to simplify user and authentication management to software developers who work on internal projects and services.

### Network computing

In the field of network computing technology and infrastructure, including high-throughput computing, high-performance computing, grids and clouds (ICT as a service), the NIC is collaborating with individual computing clusters at the institute and contributing directly to the Slovenian National Grid Initiative SLING as a funding member and core partner. The NIC maintains the Slovenian certification agency SLING CA for science, research and grid computing, takes part in the maintenance and support of the core national grid network services and coordinates work with international infrastructure projects and collaborations.

In 2014, we continued with our support for users of JSI clusters and supported the integration of the clusters with the national network SLING using the NorduGrid ARC Grid Middleware to enable users to use all the resources in the network with the same interfaces and in the same way. The upgrading of the cooling system in our data centre allowed the last turn of computing upgrades before the infrastructure is moved into the new data centre.

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**The constant growth of network services and network computing provides better support for collaboration and teamwork, software development, data protection and access to large computing and data resources for scientific research. Integration in European networks, such as EGI, provides our users with access to large international computing centres.**

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Figure 3: Observium displaying data transfer rates on one of the new routers in the core JSI network.

In the domain of network computing we have been most involved with the Slovenian National Grid Initiative (SLING), but we also worked with the European Grid Initiative EGI (with the development of the EGI Federated Cloud pilot – federated infrastructure as a service), the NorduGrid ARC collaboration and a number of international projects (ATLAS – dedicated link, Belle2 – computing grid network support planning, CLARIN – support for the creation of Slovenian national node, ELIXIR – establishment of the national node and the collaboration). SLING has supported a number of research projects and applications in 2014, among others in high-energy physics, medical sensor and image analysis, theoretical physics, astrophysics, biochemistry, protein-folding simulations, crystal analysis, knowledge technologies, statistical analysis and fluid dynamics, computational linguistics etc. In a number of cases we have been involved as part of the SLING support group in the parallelization and preparation of computing tasks and the administration of required run-time environments.

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## R & D GRANTS AND CONTRACTS

1. Slovenian Literature in Unknown Early Modern Manuscripts: Information-Technology Aided Analyses and Scholarly Editions  
Jan Jona Javoršek, B. Sc.

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## STAFF

### Technical officers

1. Vladimir Alkalaj, M. Sc., Head
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*International Multiconference Information Society - IS 2014, October 9th - 10th, 2014, Ljubljana, Slovenia: volume G, Tomaž Erjavec, ed., Jerneja Žganec Gros, ed., Ljubljana, Institut Jožef Stefan, 2014, pp. 19-24.*

# SCIENCE INFORMATION CENTRE

# SIC

*The Jožef Stefan Institute Science Information Centre is the central Slovenian physics research library and one of the largest research 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 for the Institute's staff, as requested by the funding ministry.*

Our collection of over 100,000 publications covers the fields of physics, chemistry, biochemistry, electronics, information science, artificial intelligence, nuclear technology, energy management and environmental science. We provide access to over 2500 electronic journals. We are a founding member of the ScienceDirect, SpringerLink, Wiley online library, IEEEExplore and ACS consortia. We subscribe to the SCOPUS, INSPEC and Web of Science databases, and to the SciVal research evaluation and management tool.

We manage bibliographic data for approximately 700 researchers. Our bibliographic database, which is a part of the COBISS system, contains about 80,000 records, going back to the Institute's inception in 1949. Last year's data is included as part of this report.



Head:

**Dr. Luka Šušteršič**

## NEW CONTRACT

1. Consortium Agreement for Electronic Journals Procurement for 2014  
Dr. Luka Šušteršič  
Central Technological Library

## STAFF

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5. Katarina Modic, B. Sc.
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7. Jože Škulj
8. Branka Štrancar
9. Nada Tratnik
10. Saša Žnidar





# ENERGY EFFICIENCY CENTRE

EEC

*The basic activities of the Energy Efficiency Centre are in the efficient use of energy, long-term planning in energy and the reduction of greenhouse-gases emissions. The centre is a focal point for the collection and transfer of energy-efficiency technologies to energy users, the state, energy service and equipment providers, and other interested agencies. At the same time it covers the environmental effects of energy use and conversion. The most significant part of the EEC's activities is thus its cooperation with state institutions in the preparation of strategic documents and legislation in the field of efficient energy use, energy planning, distributed electricity production, emission trading; nevertheless, it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as being increasingly involved in European research projects.*



Head:  
**Stane Merše, M. Sc.**

## Energy and the environment

In 2014 the Energy Efficiency Centre, with its professional work, ensured high-quality support to ministries in the preparation of development strategic documents and the transfer of EU legislation in the field of energy planning, energy efficiency, the use of renewables and greenhouse-gases emissions and other pollutant-reduction strategies.

The accepted EU climate-energy package set new, ambitious goals for Slovenia regarding an increase in energy efficiency, the exploitation of renewables and the reduction of greenhouse-gases emissions. Efficient energy use is a priority field for achieving these goals, in accordance with the requirements of the European Commission and the new directive on energy efficiency (2012/27/EU). According to this directive an Action Plan for Energy Efficiency for the period 2014–2020 was elaborated for the Ministry of Infrastructure together with a report on the execution of the previous plan. The EEC also cooperated in the updating of the Action Plan for Renewable Energy Sources for the period 2010–2020.

The center cooperates with the Statistical Office of the Republic of Slovenia, where it prepares a model calculation of fuels and energy use in households for the national energy statistics.

Also in 2014, the center continued with activities of the state referential centre for energy by preparing an expanded set of indicators for energy and the environment, as well cooperating in the carrying out of research on energy efficiency REUS in the public and services sector.

In the field of reducing greenhouse-gases emissions, the centre elaborated for the Ministry of Agriculture and Environment strategic studies for the establishment of a system for monitoring the carrying out and the evaluation of measures efficiency for the Operational Programme of GHG Emissions Reduction in the period 2013–2020. The EEC also continued with professional support regarding the design of goals and the national policy concerning pollutants from the NEC directive up to the year 2030.

## Promotion of efficient energy use and energy consulting

In 2014 the Energy Efficiency Centre continued with its training activities where the sixth cycle of energy-managers training was successfully concluded within the European programme EUREM. In the autumn, the seventh cycle of training had already started. Due to the very positive reactions of the participants and their interest (in Slovenia there are already more than 150 energy managers with a EUREM licence), it is clear that there is a great need for such training. High-quality knowledge in this field is of key importance for the execution of efficient solutions in practice.

In 2014 the Center of Energy Efficiency carried out several consulting tasks in the industry and public sectors. In particular, our cooperation with Luka Koper was strengthened. Great economic effects with a reduction of

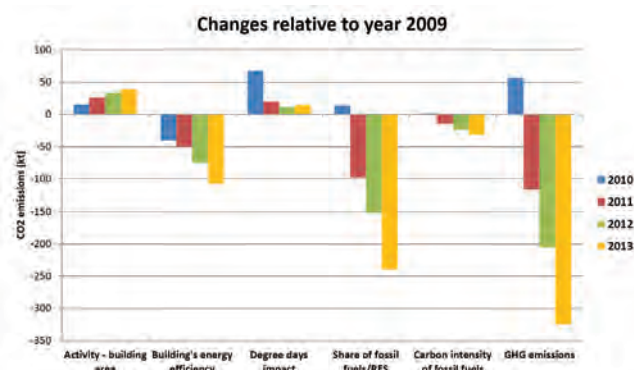


Figure 1: Decomposition analysis of the factors influencing greenhouse-gases emissions in buildings



Figure 2: Awarding certificates to the seventh generation of energy managers who concluded their EUREM training



Figure 3: LifeSaver representation of the energy consumption per day using the operator's working shift as a context variable (contour diagram)

**The research and development work of the Energy Efficiency Centre is an important contribution to the preparation of key documents in Slovenia in the field of energy development, energy efficiency, renewables exploitation and the transition of Slovenia to a low-carbon society, with training activities and support to industry it significantly contributes to an increase of competitiveness and development restructuring.**



Figure 4: The center cooperated in the carrying out of the integrated energy renovation of the four largest buildings and a heating system at the JSI Reactor Centre in Podgorica, which took place in 2014.

energy-use costs were achieved by the execution of more in depth energy audits of individual terminals and by an analysis of the possibilities for the introduction of advanced technologies of trans-loading. Professional cooperation with Salonit Anhovo, Termoelektrarna toplarna Ljubljana, BTC, General Hospital Brežice, Klinika Golnik, etc. were continued.

The Center continued its professional cooperation with the company Petrol d.d. in carrying out the biggest programme of large consumers for ensuring energy savings of the end users. The Center prepared the programme for the sixteenth conference "Energy Managers Days", the annual meeting of energy managers with more than 200 participants confirms the quality and public profile of the EEC's professional work.

#### International cooperation

In 2014 the EEC carried out as many as 14 international projects, financed from the European Union resources in the framework of the 7th Framework Programme and European Commission programme "Intelligent Energy for Europe" as well as the regional programmes MEDITERAN and Central and South East Europe.

Projects cover activities in the fields of:

- development of innovative systems for energy-use monitoring and management in industry (Life Saver, 7th FP),
- increase of energy efficiency of existing non-residential buildings with the introduction of the cost-effective optimization of energy systems Re-Commissioning (Re-Co),
- analysis of the impacts of the introduction of smart energy measurements on the use and costs of energy in low-income housing (Elih-MED),
- inclusion of the criteria of energy efficiency in public tenders (EFFECT),
- increase of the transparency of markets with energy services (Transparens)
- compiling and elaboration of current data on renewable energy sources use (EurObserv`ER Barometer),
- monitoring and promotion of cogeneration development (CODE2),
- carrying out of an EU directive on energy efficiency (CA - EED),
- carrying out of an EU directive on renewable energy sources (CA - RES),
- monitoring of indicators for energy use and energy efficiency in the EU (ODYSSEE MURE EU-27).
- development and carrying out of integrated energy concepts in technological centres (Go ECO)
- central environment energy management as a tool for survival (CEEM)
- advanced financial platform for the promotion of green growth and eco-innovations (Ecofunding)
- strengthening of policies of urban sustainability (UrbanEmpathy)
- strengthening of Mediterranean incentives which direct small and medium-sized enterprises towards innovations concerning the development of energy-efficient technologies (EMILIE)

The projects include 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 EEC staff took part in numerous foreign professional meetings and visits.

#### Some outstanding achievements in the past year

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 2020).

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, TE-TOL, Luka Koper, Salonit Anhovo, Telekom Slovenije, BTC, ELENA – Ljubljana, etc.).
3. Cooperation in different international projects in the framework of European Commission programmes in the fields of energy efficiency, energy management, combined production of electricity and heat, promotion of energy-efficient technologies and energy services, exploitation of wood biomass and others.

## Organization of conferences, congresses and meetings

1. Efficient energy renovation of public and multi-apartment buildings, Dol pri Ljubljani, 31 January 2014
2. Re-Commissioning – Raising energy performance in existing non-residential buildings, Ljubljana, 6–7 March 2014
3. Optimization of energy systems operation in the General Hospital Brežice, Brežice, 26 March 2014
4. Environment footprint of agriculture and food processing industry, Ljubljana, 27 March 2014
5. Support to the energy efficiency in industry and small and medium enterprises, Ljubljana, 28. March 2014
6. Energy managers days 2014 – 16. Meeting of energy managers of Slovenia, Portorož, 15– 16 April 2014
7. Capitalisation meeting of the project EMILIE, Ljubljana, 12 June 2014
8. Fifth project meeting CODE 2, Ljubljana, 11– 12 June 2014
9. Fifth project meeting of Urban Empathy, Ljubljana, 17– 18 September 2014
10. Seminar for decision makers in the field of sustainable urban policies: How to increase usefulness of results of ETS projects?, Ljubljana, 14 November 2014

## INTERNATIONAL PROJECTS

1. 7FP - LifeSaver; Context Sensitive Monitoring of Energy Consumption to Support Energy Savings and Emission Trading in Industry  
Boris Sučić, M. Sc.  
European Commission
2. Re-Co; Re-Commissioning-Raising Energy Performance in Existing Non-Residential Buildings  
Barbara Petelin Visočnik, M. Sc.  
European Commission
3. EFFECT - Upgrading of Energy Efficient Public Procurement for a Balanced Economic growth of SEE Area  
Polona Lah, B. Sc.  
Agenzia Regionale per L'Energia
4. ELIH-Med - Energy Efficiency in Low-Income Housing in the Mediterranean  
Aleš Podgornik, M. Sc.  
Joint Technical Secretariat MED Programme
5. Go ECO; Development and Implementation of Integrated Energy Concepts in Business Parks  
Peter Bevk, B. Sc.  
European Commission
6. CEEM - Central Environmental and Energy Management as a Kit for Survival  
Matevž Pušnik, M. Sc.  
City of Vienna, Department for EU-Strategy
7. EIE - C.O.D.E. 2; Cogeneration Observatory and Dissemination Europe 2; IEE/11/910/SI2.615940  
Stane Merše, M. Sc.  
European Commission
8. EIE pr. - TRANSPARENSE; Increasing Transparency of Energy Services Markets  
Damir Staničič, M. Sc.  
European Commission
9. EIE - ODYSSEE MURE 2012; Monitoring of Energy Efficiency in the EU  
Dr. Fouad Al-Mansour  
European Commission
10. MED - EMILIE; Enhancing Mediterranean Initiatives Leading SMEs to Innovation in Building Energy Efficiency Technologies  
Stane Merše, M. Sc.  
STC Programme MED
11. MED pr.; ECOFUNDING; Innovative Funding Scheme for Energy and Eco Innovation Projects  
Polona Lah, B. Sc.  
Provence-Alpes-Côte D'Azur Region
12. IEE; EurObserv'ER, The EurObserv'ER Barometer (2013-2016)  
Matjaž Česen, B. Sc.  
European Commission
13. URBAN EMPATHY - Empowering Policies on Urban Sustainability  
Aleš Podgornik, M. Sc.  
Provence-Alpes-Côte D'Azur Region

## RESEARCH PROGRAM

1. Modelling and Environmental Impact Assessment of Processes and Energy Technologies  
Dr. Fouad Al-Mansour

## NEW CONTRACTS

1. Concerted Actions in the Field of the Directive on End Energy Efficiency (CA EED II)  
Damir Staničič, M. Sc.  
Ministry of Infrastructure
2. Energy Efficiency Obligation Scheme for Large Energy Sales Companies  
Damir Staničič, M. Sc.  
Petrol d. d., Ljubljana
3. Elaboration of a Concept and Methodology of the Research of Energy Efficiency of Slovenia for the Public and Services Sector  
Stane Merše, M. Sc.  
Informa Echo, d. o. o.
4. Development Project for Establishing a Platform of Advanced Services for Energy Management of Household Consumers  
Aleš Podgornik, M. Sc.  
Solvera Lynx, d. d.
5. National Reference Centre for Energy and Refreshment of Energy and Environment Indicators 2013/14  
Matjaž Česen, B. Sc.  
Ministry of the Environment and Spatial Planning
6. Updating of Energy Balances and Strategic Studies for the Determination of National Energy Goals  
Andreja Urbančič, M. Sc.  
Ministry of Infrastructure
7. Validation and Transfer of Technologies, EU Project GreenBerth - Design of the Methodology for the Validation and Transfer of Technologies relevant for Energy Efficiency Improvements in Ports' Operations  
Boris Sučić, M. Sc.  
Luka Koper, d. d.
8. Allocation of Financial Means and Cooperation in the European Project Concerted Action in the Field of the RES II directive  
Damir Staničič, M. Sc.  
Ministry of Infrastructure
9. Action Plan for Energy Efficiency and Reporting on its Carrying Out  
Damir Staničič, M. Sc.  
Ministry of Infrastructure
10. Strategic Studies for the Revision of the NEC Directive  
Matjaž Česen, B. Sc.  
Ministry of the Environment and Spatial Planning
11. Professional Support and Consulting for the Preparation of the Third Party Financing on Pilot Projects of the Community Brda according to ESCO model (MARIE project)



- Damir Staničič, M. Sc.  
Golea, Nova Gorica
12. 16th Meeting of Slovenian Energy Managers - Energy Managers Days 2014  
Stane Merše, M. Sc.  
Časnik Finance, d. o. o.
13. Establishment of the Monitoring System of Carrying Out and Evaluation of Efficiency Measures with the Impact on GHG Emissions Motion  
Andreja Urbančič, M. Sc.  
Ministry of the Environment and Spatial Planning
14. Framework Agreement on the Professional Advising in the Field of Cogeneration  
Stane Merše, M. Sc.  
Energetika Ljubljana, d. o. o.
15. Elaboration of a Report on Achieving of National Framework Goals in the Field of RES and CHP for the Period 2012 - 2014  
Andreja Urbančič, M. Sc.  
The Energy Agency

## VISITORS FROM ABROAD

1. Johan Coolen, Factor4, Antwerp, Belgium, 6-7 March 2014
2. Stefan Plessner, EDB, Braunschweig, Germany, 6-7 March 2014
3. Esa Nykaenen, VTT, Espoo, Finland, 6-7 March 2014
4. Bohuslav Malek, SEVEN, Prague, Czech Republic, 6-7 March 2014
5. Boris Papousek, direktor, Graz Energy Agency, Graz, Austria, 6-7 March 2014
6. Reinhard Ungerböck, Graz Energy Agency, Graz, Austria, 6-7 March 2014
7. Mirjana Prljević, president of Teslium, Belgrade, Serbia, 11 July 2014
8. Boris Vukobrat, president of Peace and Crises Management, Paris, France, 11 July 2014
9. Marko Voljč, member of the executive committee KBC, Brussels, Belgium, 11 July 2014

## STAFF

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  9. Marko Pečkaj, B. Sc.
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  11. Aleš Podgornik, M. Sc.
  12. Boris Sučić, M. Sc.
- Technical and administrative staff**
13. Peter Bevk, B. Sc.
  14. Roza Pergarec, B. Sc.
  15. Igor Ribič

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3. Matevž Pušnik, Boris Sučić, "Integrated and realistic approach to energy planning - a case study of Slovenia", *Management of environmental quality*, iss. 1, vol. 25, pp. 30-51, 2014.
4. Matevž Pušnik, Boris Sučić, Fouad Al-Mansour, Luigi Crema, Marco Cozzini, Shahriar Mahbub, Christoph Holzner, Johannes Kohlmaier, "Framework for sustainability assessment of small and medium-sized enterprises", *Chem. Eng. Trans.*, vol. 42, pp. 121-126, 2014.
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2. Fouad Al-Mansour, Boris Sučić, Matevž Pušnik, Tomaž Vuk, "Novel concept of context sensitive energy and environmental management system for support sustainable development of industrial companies", In: *Proceedings: Retool for a competitive and sustainable industry*, ECEEE Industrial Summer Study, Retool for a competitive and sustainable industry, 2-5 June 2014, Stockholm, Stockholm, ECEEE, 2014, pp. 239-246.
3. Viktor Jejič, Fouad Al-Mansour, "Ogljični odtis konvencionalne in ekološke poljedelske pridelave", In: *Aktualni zadaci mehanizacije poljoprivrede: Zbornik radova 42. Međunarodnog simpozija iz područja*

- mehanizacije poljoprivrede, Opatija, 25. - 28. veljače 2014: proceedings of the 42nd International Symposium on Agricultural Engineering, Opatija, Croatia, 25-28 February 2014*, (Actual tasks on agricultural engineering, 42), 42. Međunarodni simpozij iz područja mehanizacije poljoprivrede, Opatija, 25. - 28. veljače 2014, Silvio Košutić, ed., Zagreb, Sveučilište u Zagrebu, Agronomski fakultet, Zavod za mehanizaciju poljoprivrede, 2014, f. 447-457.
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  5. Maria Marques, Boris Sučić, Tomaž Vuk, "Context-based decision support for sustainable optimization of energy consumption", In: *SDM'2014*, Rossitza Setchi, ed., et al, Cardiff, KES International, 2014, pp. 899-910.
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  9. Matevž Pušnik, Boris Sučić, Aleš Podgornik, Fouad Al-Mansour, Tomaž Vuk, "Net fitting based production planning and decision support system for energy intensive industries", In: *Energycon 2014*, [Zagreb, Faculty of Electrical Engineering and Computing], 2014, pp. 1236-1242.

10. Boris Sučić, Fouad Al-Mansour, Matevž Pušnik, "A linear programming approach for production planning optimisation and peak load management in industrial companies", In: *SEEP*, 7th International Conference on Sustainable Energy and Environmental Protection, SEEP [2014], Dubai - UAE, November 23-25, 2014, Dubai, The British University, University of the West Scotland, 2014, 6 pp.
11. Boris Sučić, Fouad Al-Mansour, Matevž Pušnik, Tomaž Vuk, "Concept of an integrated performance measurement system in energy intensive industries: Energy and environmental indicators", In: *Digital proceedings*, (CD Proceedings), 1st South East European conference on

sustainable development of energy, water and environment systems, 29 June - 3 July 2014, Ohrid, Marko Ban, ed., et al, Ohrid, 2014, 11 pp.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Aleš Podgornik, Boris Sučić, Damir Staničić, "Smart metering and sustainable behavior in low-income households in the Mediterranean", In: *Handbook of climate change adaptation*, Walter Leal Filho, ed., Berlin, Springer-Verlag, 2014, 22 pp.



# CENTRE FOR ELECTRON MICROSCOPY AND MICROANALYSIS

# CEMM

*The Centre for Electron Microscopy and Microanalysis (CEMM) is a JSI instrumental centre that was founded on 1 January 2014 as an upgrade of the previously existing Center for Electron Microscopy. The CEMM comprises the research equipment for electron microscopy that is necessary for the research work of the JSI departments. Other research institutes, universities and industry also have access to the equipment. The users of the CEMM equipment are the researchers in the field of materials science that are involved in chemical and structural analyses of materials on the micro and atomic scales. The major equipment of the CEMM represents three scanning electron microscopes (JSM-5800, JSM-840A, JSM-7600F), two transmission electron microscopes (JEM-2100 (CO NiN) and JEM-2010F) and sample-preparation equipment. Additionally, CO NAMASTE upgraded the equipment of the Centre with a CCD camera for the JEM-2010F, an ADF detector for the JEM-2010F and an EBSD system for the JSM-7600F.*



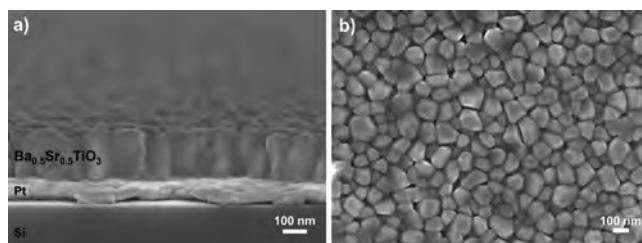
Head:  
**Prof. Miran Čeh**

Scanning electron microscopy (SEM) is used for morphological studies of either fractured or polished surfaces. Since all scanning electron microscopes are equipped with the X-ray spectroscopy (EDXS and/or WDXS), qualitative and quantitative chemical analysis on the micro scale are also possible. Since only a few  $\mu\text{m}^3$  of the material are non-destructively analysed, 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 back-scatter diffraction (EBSD) and electron lithography.

When structural features on the nano-scale are investigated, however, various techniques of the transmission electron microscopy (TEM) are used. The JEM-2010F with a FEG (field-emission gun) is equipped with a STEM unit, EDXS, EELS and CCD camera, while the JEM-2100 is equipped with EDXS and a CCD camera. The CEMM also comprises the equipment for SEM and TEM specimen preparation, which is the first starting point for all electron microscopy observation procedures. Especially important are the high- and low-energy ion-mills, which enable the preparation of thin foils that are transparent for high-energy electrons, and a tripod polisher for the mechanical thinning of the samples.

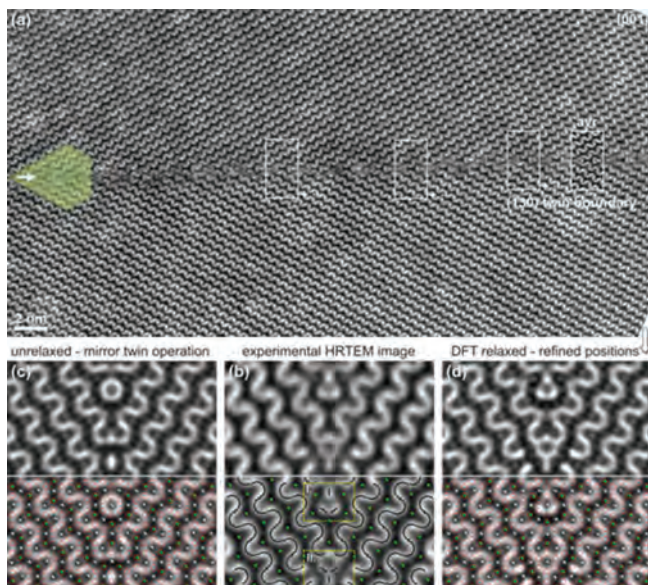
The analytical work that is performed on the CEM equipment varies, concerning both the investigated materials and/or the used electron microscopy techniques. While the scanning electron microscopy is used mainly for microstructural characterization and the chemical analysis of polycrystalline ceramic materials (functional ceramics, engineering ceramics, bio-ceramics, and composites), magnetic materials, glasses, metals, alloys, etc., the transmission electron microscopy is used for structural and chemical investigations of grain boundaries, planar faults, dislocations and precipitates within the same materials. The structural and chemical analysis of the grain boundaries is especially important since it is known that the final physical properties to a great extent depend on the structure and the chemistry of the grain boundaries.

One of the main tasks of the CEMM staff is to maintain the equipment in optimal working condition. Other activities of the CEMM include training for operators, service type of work and the implementation of new electron-microscopy analytical methods.

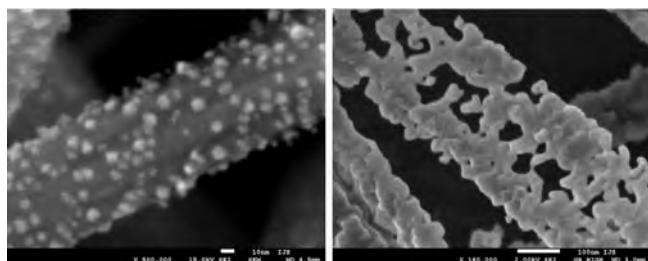


*Figure 1: FE-SEM micrographs of a) cross-section and b) surface microstructures of  $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$  thin film deposited on a platinized silicon substrate by chemical solution deposition and rapid thermally annealed at  $900\text{ }^\circ\text{C}$ . The film consists of predominantly columnar grains, as is evident from the cross-section image. The average lateral grain size is around  $80\text{ nm}$ . Thin-film capacitors based on  $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$  with a Curie temperature of  $\sim 250\text{ K}$ , have been investigated for applications in the microwave range, such as tunable phase shifters or filters, due to the ability to change their dielectric permittivity with an external electric field. Electronic Ceramics: Tanja Pečnik*

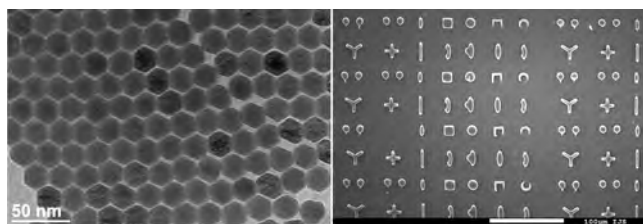




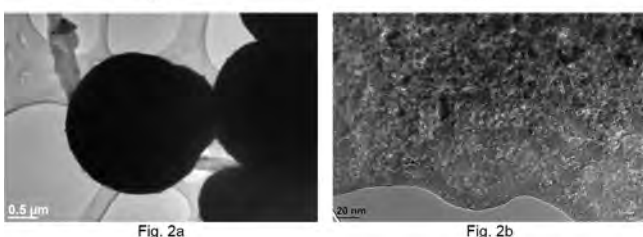
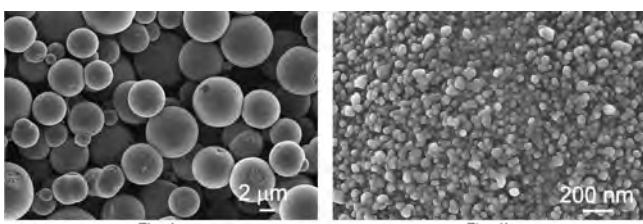
**Figure 2: (130) twin boundary in chrysoberyl.**  
 A HRTEM study of the (130) twin boundary in chrysoberyl using a conventional 200 kV JEM 2100 microscope. (a) Unprocessed experimental HRTEM image. The twin boundary is not straight, but climbs from left to right by making  $\frac{1}{2} \cdot d_{130}$  steps to the adjacent (260) planes. In straight sections, the boundary shows periodic features along the interface (see outlined super-cells). A series of periodic cells was used to produce an average experimental image with enhanced contrast (see the last inset of the series; avr). (b) A close-up of the processed experimental image. In the lower part of the image wavy chains are produced by undulating O-columns (outlined by black ripples). The black areas in between correspond to the positions of the Be-columns (green dots). I and II denote two unique atomic clusters along the interface. (c) The simulated HRTEM image based on the rigid atomic model produced by mirror operation over an (130) lattice plane with overlaid atomic positions (O - red, Al - grey, Be - green). (d) Simulated HRTEM image based on a DFT refined atomic model with shifted Be and O atoms in Cluster-I, and displaced Be atoms to the neighbouring tetrahedral sites in Cluster-II. Reference: Sandra Drev, Matej Komelj, Matjaž Mazaj, Nina Daneu and Aleksander Rečnik. Structural investigation of (130) twins and rutile precipitates in chrysoberyl crystals from Rio das Pratinhas in Bahia (Brazil). *American Mineralogist* 100/4 (2015) in press. Nanostructured materials: Sandra Drev



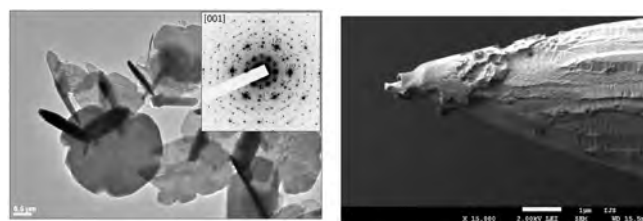
**Figure 5: Corn nanocob: WO<sub>3</sub> nanoribbons decorated with Au nanoparticles.** Material was synthesized by AACVD (aerosol assisted chemical vapor deposition) technique.  
 Nanolace: Titanium oxynitride nanoribbons prepared by calcination of protonated titanate nanoribbons in NH<sub>3</sub>(g).  
 Condensed Mater Physics: Polona Umek, Melita Rutar



**Figure 3: Self-assembled NaYF<sub>4</sub> nanoparticles (Jeol 2100).** Magnetic PDMS particles (sSPIONs™ | PDMS, company Nanos SCI Ltd) micro-fabricated by photolithography (Jeol 7600F).  
 Synthesis of Materials: Darja Lisjak



**Figure 4: Nanostructured spherical anatase particles with sizes ranging from 2 to 7 nm** were prepared by solvothermal synthesis with different processing parameters (Fig. 1a). The materials exhibit interesting photocatalytic activity under UV light. The size of the primary crystallites that was determined based on the XRD analysis by applying the Scherrer equation was from 10 to 20 nm, which is in agreement with the FESEM analysis (Fig. 1b). The materials exhibit a high specific surface area up to 208 m<sup>2</sup>g<sup>-1</sup>. The particles of the as-prepared materials cannot be analysed by TEM analysis, due to their, relatively large size (Fig. 2a). However, by mixing the particles in epoxy resin and thinning such specimens down to few nm one can study their internal mesoporous structure (Fig. 2b).  
 Advanced Materials: Srečo Škapin



**Figure 6: Strontium hexaferrite crystals (SrFe<sub>12</sub>O<sub>19</sub>):** thin tabular Sr-HF crystals are synthesized in μm sizes but only few nm thick, thus transparent for the electrons and suitable for observation in a transmission electron microscope. The TEM micrograph and SAED was made on Jeol JEM-2100 with LaB<sub>6</sub> electron source. (Material: Petra Jenuš K7): Tungsten tip prepared by electrochemical etching in NaOH solvent, for Scanning Tunneling Microscopy. (Material: Andrej Kranjec F7)  
 Centre for Electron Microscopy and Microanalysis: Janez Zavašnik, Maja Češarek

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# 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 2014 the centre was active in several European projects from FP7: *RENDER (Reflecting Knowledge Diversity)*, *PLANETDATA (A European Network of Excellence on Large-Scale Data Management)*, *TRANSLECTURES (Transcription and Translation of Video Lectures)*, *X-LIKE (Crosslingual Knowledge Extraction)*, *MOBIS (Personalized Mobility Service for energy Efficiency and Security through Advanced)*, *MEDIAMIXER (Community Set-up and Networking for the Remixing of Online Media Fragments)*, *NRG4CAST (Energy Forecasting)*, *SOPHOCLES (Self-Organised information Processing, Criticality and Emergence in multile)*, *CENTRAL COMMUNITY (Emerging communities for collective innovation in Central Europe)*, *SYMPHONY (Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy)*, *X-LIME (crossLingual crossMedia knowledge extraction)*, *PROASENSE (The Proactive Sensing Enterprise)*.

In 2014 the centre was active in 12 European projects. The centre prepares and organizes educational events, such as conferences, seminars, workshops, and summer schools. These events are targeted at experts who would like to apply the latest knowledge and achievements from intelligent data analysis, knowledge technologies, data mining, text mining and decision support to the areas of network organizations, business decisions, finance, marketing, automation and process control. A special consideration is put on the managers and decision makers who are aware of the strengths and benefits to the success of their businesses.

All educational events are designed to transfer basic, additional and the 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://videlectures.net/>. It now offers more than 20,000 recorded tutorials from different scientific events and is visited every month by an average of 135,000 visitors from around the world. The main purpose of the portal is to provide free and open access to high-quality video lectures presented by distinguished scholars and scientists at the most important and prominent events. In today's world, VideoLectures.NET represents a free knowledge hub, a way of opening up education to everyone, as there is a great need to share educational content at all levels in order to benefit society and foster the economy. It also gives a learning opportunity to audiences at all social levels.

We have successfully collaborated within the Videlectures.net portal with some of the top ten American universities MIT (Massachusetts Institute of Technology), University of California - Berkeley, YALE, John Hopkins University, University of California, Irvine, and Carnegie Ethics Studio, as well as with the European CERN and ETH from Zurich. VideoLectures.Net has strong connections in OpenCast Foundation, OpenCourseWare Consortium and Knowledge 4 All Foundation Ltd.

The centre also operates a web portal <http://www.ist-world.org> that offers services for automatic data collection and an analysis of European research. The user can perform several simple and complex analyses, predictions and detect trends in research. This is an exceptional web service that is being visited daily by an average of 6,000 unique visitors.



Head:  
**Mitja Jermol, M. Sc.**

**In 2014 the Centre for Knowledge Transfer in IT was actively involved in 12 European projects.**



Figure 1: Signing the agreement of the establishment of a UNESCO Chair on Open Technologies for Open Educational Resources and Open Learning

**CT3 is operating web portal <http://videlectures.net/>, which is now the largest world reference portal presenting high-quality scientific lectures.**





Figure 2: Global conference OCWC was held in April 2014 in Ljubljana.

In 2014 we organized the 9th Student Competition in Computer Science, attended by 129 students from Slovenian secondary schools. We have also organized project meetings for different EU projects (NRG4CAST, Xlime, Symphony, Sophocles and X-LIKE) and an international conference, supported by the EU project TRANSLECTURES, MediaMixer and X-like “OCWC Global Conference”, which was attended by 250 experts.

Following the success of VideoLectures.NET, recognized by the UN and UNESCO as one of the most outstanding examples of creative and innovative e-Content in the world in the past decade, the “Jožef Stefan” Institute has successfully established a UNESCO Chair on Open Technologies for OER and Open Learning. The Chair is currently expanding its vision and strategy in collaboration within OpeningupSlovenia and with the Knowledge 4 All Foundation Ltd based in London, UK.

With this prestigious title, the Jožef Stefan Institute has proven that its vision of free and open access to academic knowledge in the form of open online videos and smart technologies is the right approach for addressing the

global digital divide in education and knowledge transfer. The Chair on Open Technologies for Open Educational Resources and Open Learning is operating with an initial set of assets in the form of the EU FP7 research projects transLectures, MediaMixer, xLiMe, XLike, and VideoLectures.Net, an award-winning video library. Its work is in synergy with the OpeningupSlovenia initiative and the Knowledge 4 All Foundation Ltd, dedicated to the creation of tools and intelligent services in open education.

The Chair Mitja Jermol, M.Sc. is serving to promote an integrated system of research, training, information and documentation on online learning for Open Educational Resources (OER) and open learning. It is facilitating collaboration between high-level, internationally recognized researchers and teaching staff of the Institute and other institutions around the world.

## Organization of conferences, congresses and meetings

1. 9<sup>th</sup> Student competition in computer science, Ljubljana, 29. 3. 2014
2. Organization of the international conference “OCWC Global Conference” Ljubljana 22.-25.4. 2014

## INTERNATIONAL PROJECTS

1. Video recording and post production  
Mitja Jermol, M. Sc.  
Foreign buyers
2. 7FP - PlanetData  
Mitja Jermol, M. Sc.  
European Commission
3. 7FP - X-Like; Cross-lingual Knowledge Extraction  
Mitja Jermol, M. Sc.  
European Commission
4. 7FP - transLectures; Transcription and Translation of Video Lectures  
Mitja Jermol, M. Sc.  
European Commission
5. 7FP - MobiS: Personalized Mobility Services for Energy Efficiency and Security through Advanced Artificial Intelligence Techniques  
Mitja Jermol, M. Sc.  
European Commission
6. 7FP - Sophocles; Self-Organised information Processing, Criticality and Emergence in multilevel Systems  
Marjana Plukavec, B. Sc.  
European Commission
7. 7FP - MEDIAMIXER; Community Set-up and Networking for the Remixing of Online Media Fragments  
Mitja Jermol, M. Sc.  
European Commission
8. 7FP - NRG4CAST; Energy Forecasting  
Mitja Jermol, M. Sc.  
European Commission
9. 7FP - xLiMe; CrossLingual CrossMedia Knowledge Extraction  
Mitja Jermol, M. Sc.  
European Commission
10. 7FP - SYMPHONY; Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy  
Mitja Jermol, M. Sc.  
European Commission
11. 7FP - ProaSense; The Proactive Sensing Enterprise  
Mitja Jermol, M. Sc.  
European Commission
12. 7FP - SUNSEED; Sustainable and Robust Networking for Smart Electricity Distribution  
Mitja Jermol, M. Sc.  
European Commission
13. 7FP - FI-IMPACT; Future Internet Impact Assurance  
Mitja Jermol, M. Sc.  
European Commission
14. CE - Central Community-Emerging Communities for Collective Innovation in Central Europe  
Mitja Jermol, M. Sc.  
City of Vienna, Department for EU-Strategy

## R & D GRANTS AND CONTRACTS

1. Cloud Assisted Services: CC CLASS  
Mitja Jermol, M. Sc.
2. ExplorEdu - a system of open and available web services and mobile applications for automatic identification of OER  
Mitja Jermol, M. Sc.
3. International Conference OCWC Global Conference 2014, Ljubljana, Slovenia, 21-25 April 2014  
Tanja Zdolšek, B. Sc.

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4. Marjana Plukavec\*, B. Sc.
5. Špela Sitar, B. Sc.

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8. Ana Fabjan, B. Sc.
9. Goran Kodrun
10. Adis Krečo, B. Sc.
11. Monika Kropelj, B. Sc.
12. Davor Orlič, B. Sc.
13. Tanja Zdolšek, B. Sc.

Note:

\* part-time JSI member

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1. Tanja Zdolšek, Karin Širec, "Proučevanje vpliva podjetniškega izobraževanja na podjetniške namere študentov: pregled dosedanjih empiričnih raziskav", *Naše gospod. (Tisk. izd.)*, vol. 60, no. 3/4, pp. 55-64, 2014.

### PUBLISHED CONFERENCE CONTRIBUTION

1. Lyndon Nixon, Tanja Zdolšek, Ana Fabjan, Peter Kese, "Video Lectures Mashup - remixing learning materials for topic-centred learning

across collections", In: *Open education for a multicultural world: OCWC Global Conference, 23-25 April Ljubljana, Slovenia*, Ljubljana, Jožef Stefan Institute, Centre for Knowledge Transfer in Information Technologies, 2014, 15 pp..

2. Lyndon Nixon, Tanja Zdolšek, Ana Fabjan, Peter Keše, "VideoLecturesMashup: using media fragments and semantic annotations to enable topic-centred e-learning", In: *The semantic web: ESWC 2'014 satellite events: SWC 2014, Satellite Events, Anissaras, Crete, Greece, May 25-29, 2014: revised selected papers*, (Lecture notes in computer science, 8798), Valentina Presutti, ed., Cham [etc.], Springer, 2014, vol. 8798, pp. 450-454, 2014.





# MILAN ČOPIČ NUCLEAR TRAINING CENTRE

## ICJT

*The mission of the ICJT training centre is training in the field of nuclear technologies and radiation protection. In addition, the ICJT is actively informing the public about these technologies.*

Training in the area of nuclear technologies is our primary mission. The course *Nuclear technology*, which is the initial theoretical training for future control-room operators, which started in the autumn of 2014, is in its 15<sup>th</sup> edition. These courses are normally organized every second year. In spring 2014, there was also a course entitled *Basics of nuclear technology*, which is intended for the non-control-room personnel of nuclear power plants (NPPs) and participants from other organizations.

There were 28 **radiological protection training** courses for the medical, industrial and research use of radioactive sources. Two additional courses were conducted for the transport of nuclear materials and for the security personnel of Reactor Centre Podgorica.

In collaboration with the Environmental Sciences Division, there was a radiochemistry course for participants from EU candidate countries. An important result of our **international activity** is the preparation of training materials (23 modules) for the IAEA course “Basic Professional Training Course” (BPTC).

**Public information** remains an important part of our activities. Groups of visitors (mainly schoolchildren, students and various societies) were regularly attending the 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 143 groups or 6477 visitors this year. Since 1993 our information centre has been visited by a total of 155464 pupils, teachers and other visitors. We have continued monitoring and analysing media reports on nuclear energy. A one-day workshop entitled “Radioactivity and Radiation” was prepared for demonstrators in schools and science centres.



Head:  
**Prof. Igor Jenčič**

**A package of training materials (23 modules; for each of them a textbook, viewgraphs, case studies, test questions) was prepared for the “IAEA Basic Professional Training Course” on nuclear safety.**



Figure 1: Lecture at the Nuclear Power Plant (NPP) technology course



Figure 2: Exercise of trainees at the NPP simulator



Figure 3: Lecture about radioactivity for school children



Figure 4: Lecture about energy for primary-school children



Figure 5: Learning materials for IAEA

**Table of training activities at Nuclear Training Centre in 2014**

Date	Title of the course	Parti- pants	Lecturers	Weeks	Participants × weeks
6. 1.-22. 1.	Radiation protection for RP department staff	6	17	2.6	15.6
27. 1.-31. 1.	Radiation protection for RP department staff - refresher course	11	3	1	11
24. 2.-26. 2.	Radiation protection for industrial and other practices (sealed sources)	3	5	0.6	1.8
24. 2.-27. 2.	Radiation protection for industrial and other practices (radiography)	2	4	0.8	1.6
24. 2.-28. 2.	Radiation protection for industrial and other practices (measurement of roadway density and humidity)	1	4	1	1
24. 2.-26. 2.	Radiation protection for industrial and other practices (unsealed sources)	5	4	0.6	3
27. 2.-28. 2.	Radiation protection for Dental Radiography	3	5	0.4	1.2
4. 3.	Radiation protection for industrial and other practices - Refresher Course	15	4	0.2	3
4. 3.-6. 3.	Radiation protection for industrial and other practices (measurement of roadway density and humidity) - Refresher Course	1	4	0.4	0.4
4. 3.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	6	5	0.2	1.2
4. 3.	Radiation protection for industrial and other practices (radiography) - Refresher Course	6	4	0.2	1.2
4. 3.	Radiation protection for industrial and other practices (sealed sources) - Refresher Course	4	4	0.2	0.8
6. 3.	Training Extension for RP Officers	18	2	0.2	3.6
5. 5.-3. 6.	Basics of nuclear technology, theory	9	12	4.4	39.6
27. 5.	Radiation protection for industrial and other practices (min. exposed workers)	36	3	0.2	7.2
4. 6.-27. 6.	Basics of nuclear technology, systems	11	10	3.4	37.4
22. 9.	Radiation protection for exposed workers in medicine and veterinary	24	3	0.2	4.8
1. 10.	Radiation protection for Cinkarna Celje Workers - Refresher Course	10	2	0.2	2
2. 10.	Radiation protection for Cinkarna Celje Workers	4	2	0.2	0.8
6. 10.-8. 10.	Radiation protection for medical and veterinary workers	1	4	0.6	0.6
6. 10.-10. 10.	Radiation protection for industrial and other practices (sealed sources)	5	9	1	5
6. 10.- (3. 3. 2015)	Radiation protection for industrial and other practices (unsealed sources)	21	22	13	273
6. 10.-8. 10.	Nuclear Technology, Theory	3	5	0.6	1.8
6. 10.-8. 10.	Radiation protection for medical and veterinary workers - Nuclear medicine workers	11	4	0.6	6.6
6. 10.-17. 10.	Radiation protection exposed to radon and thoron	1	4	0.6	0.6
14. 10.	Radiation protection for industrial and other practices (sealed sources) - Refresher Course	4	6	0.2	0.8
14. 10.	Radiation protection for industrial and other practices (measurement of roadway density and humidity) - Refresher Course	3	4	0.2	0.6
14. 10.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	2	3	0.2	0.4

## Table of training activities at Nuclear Training Centre in 2014

Date	Title of the course	Partici- pants	Lecturers	Weeks	Participants × weeks
14. 10.	Radiation protection for Nuclear Medicine Dept. - Refresher Course	18	3	0.2	3.6
16. 10.	Training Extension for RP Officers	11	2	0.2	2.2
17. 10.	Radiation protection for Dental Radiography - Refresher Course	3	3	0.2	0.6
4. 11.-5. 11.	Security officers for the transport of nuclear materials - refresher course	12	4	0.4	4.8
10.-21. 11.	Training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC Enlargement & Integration policy	6	3	2	12
25.-26. 11.	Refresher course for Security Officers	8	10	0.4	3.2
<b>TOTAL</b>		<b>284</b>	<b>183</b>	<b>37.4</b>	<b>453</b>

## INTERNATIONAL PROJECTS

- 7FP - Fusion Expo; Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN-FUSEX  
Tomaž Skobe, B. Sc.  
Ministry of Education, Science and Sport
- 7FP - EAGLE; Enhancing Education, Training and Communication Processes for Informed Behaviors and Decision-making related to Ionizing Radiation Risks  
Rado Istenič, B. Sc.  
European Commission
- Design, Development and Delivery of Training Material for the Train-the-Trainer's Package on Nuclear Safety  
Dr. Igor Jenčič  
IAEA - International Atomic Energy Agency

## R & D GRANTS AND CONTRACTS

- Trainings of the RZ for Foreign Market  
Matejka Južnik, M. Sc.

## NEW CONTRACTS

- Implementation of the ICJT Training Programme in 2015  
Dr. Igor Jenčič  
Krško Nuclear Power Plant
- Implementation of the Training Programme "Nuclear Power Plant Technology" (TJE 2015)  
Dr. Igor Jenčič  
Gen energija, d. o. o.
- Public Information and Monitoring of Media regarding Nuclear Energy and Activities of GEN-energija  
Dr. Igor Jenčič  
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- Matjaž Koželj, "ALARA in practice", In: *Proceedings*, 23rd International Conference Nuclear Energy for New Europe - NENE 2014, Portorož, Slovenia, September 8-11, Igor Jenčič, ed., Ljubljana, Nuclear Society of Slovenia, 2014, 7 pp.





# RADIATION PROTECTION UNIT

# SVPIS

***The SVPIS has been involved in ionizing-radiation measurements and radiation protection since the commissioning of the TRIGA MARK II Research reactor in 1966. The responsibility of SVPIS is the radiation control of all the activities at the Institute dealing with ionizing radiation. Our main task is the supervision of the reactor and the 17 laboratories that use sources of ionising radiation in their research work. More than hundred different sources are used, such as sealed sources, open sources, X-ray units and the accelerator TANDETRON, which need regulatory control.***

SVPIS is authorized by the Slovenian radiation protection administration to perform control in industrial and research institutions dealing with open or sealed radioactive sources and X-ray units. Furthermore, we are involved in radioactive waste management.

The measurements of dose rate, contamination and gamma spectrometry are performed by an accredited method (EN ISO/IEC 17025).

## Personal dosimetry

The personal doses of 108 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters. The maximum individual yearly dose was 0.17 mSv. This is only 0.9 % of the regulatory limit for occupational exposure (20 mSv per year) and 17 % of the limit for the general public (1 mSv per year). The collective dose at the JSI in the year 2014 was 1.26 man mSv.

## Supervision of research reactor and laboratories

The controlled area of the Research Reactor, the Hot Cell Facility and the Department of Environmental Sciences was monitored on a weekly basis. During some activities the constant presence of a radiation-protection worker was needed (i.e., for the opening of activated samples or radioactive-waste management). Measurements of dose rate, surface contamination, contamination of different objects and personal contamination were performed routinely. In most cases, no or very low contamination levels could be measured in the controlled areas.

In 2014 we performed 17 inspections in other JSI laboratories. An independent inspection by an external authorized institution was performed in the SVPIS laboratory and two additional laboratories at the JSI. There were no deficiencies recognized that could be important for radiation protection.

At present, 108 sources of radiation are used that require regulatory control. Additionally, 399 low-activity sources are also used in different laboratories.

## Environmental measurements

The environmental monitoring of the Reactor Center was performed in accordance with the existing program. The monitoring program consists of effluent measurements and measurements of samples in the environment. Activity concentrations of gamma emitters in water samples, filters, noble gases, soil samples and sediment samples were measured periodically. About 350 different samples have been measured with gamma spectrometry. Environmental passive dosimeters have been used to monitor radiation levels in the surroundings of the reactor. Based on the effluent measurements and a conservative, environmental transfer model the effective dose to the reference group of the public was estimated to be less than 1  $\mu$ Sv/year. The public exposure in 2014 due to activities at the Reactor Center was insignificant.

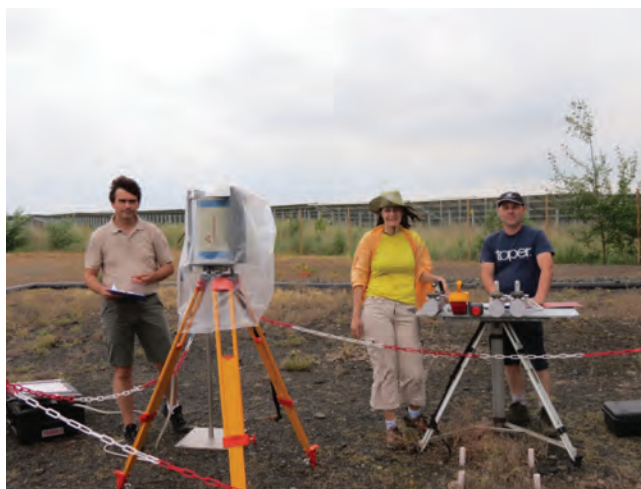
## Expert assessments and measurements for outside customers

The Radiation Protection Unit is authorized for supervision measurements and expert assessments in the field of radiation protection. In the past year several radiological control investigations were carried out in industrial



Head:

***Matjaž Stepišnik, M. Sc.***



*Figure 1: In-situ gamma spectrometry measurements and dose-rate measurements at a former uranium mine near Ronneburg*

and research institutions. Our group has participated in the evaluation of radiological monitoring of Krško NPP, research reactor TRIGA and storage for low- and intermediate-level waste in Brinje.

In the field of international cooperation our team has participated together with the Department for Low and Medium Energy Physics (F2) in intercomparison measurements at Ronneburg (Figure 1).

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### Technical and administrative staff

3. Emira Bašić, B. Sc.
4. Thomas Breznik, B. Sc.

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## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Borut Smodiš, Tinkara Bučar, Radojko Jaćimović, "Comparison of different approaches to estimate uncertainty budget in kfsbg0-INAA measurement", *J. radioanal. nucl. chem.*, vol. 300, issue 2, pp. 573-579, 2014.

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1. Milko Križman, Matjaž Stepišnik, "Historical review of exposure due to the C-14 discharges from the Krško NPP", In: *Proceedings*, 23rd International Conference Nuclear Energy for New Europe - NENE

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### INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Matjaž Stepišnik, "Reka Sava", In: *Meritve radioaktivnosti v okolju in na izviri ter njihova obravnava v luči morebitnega vpliva NEK na okolje*, Matjaž Korun, et al, 1. izd., Ljubljana, Institut Jožef Stefan, 2014, pp. 7-26.

# CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION CTT

*The Center for Technology Transfer and Innovation (CTT) has existed at the Jožef Stefan Institute since January 2011. The center's primary task is to enable and facilitate the transfer of technologies and knowledge from the JSI to the economy (contract and collaborative research, licensing, spin-out creation and associated procedures for the protection of intellectual property). We also transfer knowledge from science to the school system. The financing of CTT is based on research work in the field of innovation and innovation management – mainly through EU projects.*



Head:  
**Dr. Špela Stres, LLM**

In the OECD's opinion (October 2014), CTT is the largest and most successful technology transfer unit in this part of the EU. The center's success originates in the work of 13 professionals, 8 of which are educated in natural sciences and engineering, 5 in economics, 2 in law and 2 in social sciences, while one of the experts is also qualified as a patent attorney. We are members of the ASTP (Association of European Science and Technology Transfer Professionals) and the LES (Licensing Executives Society), in 2014 we acquired the U.S. certificate "Certified Licensing Professional". Additionally, in 2014, we have been invited to present our concept in Turkey, Poland, Croatia and Serbia, at the WIPO's Regional Workshop and to the European Commission in Brussels.

We are active in the field of technology and knowledge transfer, while our key tools are exceptional networking capability, leading to links between researchers and companies from all technology sectors (we have connections with 5,110 Slovenian and 84,852 foreign companies, maintain a network of TT coordinators within the JSI and are included in the operation of such a network at the University of Ljubljana), and consistent professionalism in conducting all the procedures – from the first contact, communication with the parent institution (the source of intellectual property), communication with the company regarding its needs, preparation of market offers, passive and active marketing, to the preparation of negotiation positions, conducting the negotiations and preparation of various contracts. Our goal is to ensure that the agreements protect the possibility of the invention's commercialization, reducing the possibility of unnecessary tensions and misunderstandings between researchers and businesspersons that block the invention's path to the market.

The unit is financially independent, meaning that the researchers are not charged for the services rendered by the CTT. Moreover, our services are free of charge also for companies that collaborate with the researchers. No funding is dedicated for the activities we perform (and for the performance of which we were established), neither in Slovenia in general nor at the JSI in particular, which forces us to finance our day-to-day existence through research and analysis work in the field of innovation and innovation management, performed mainly in the course of various EU projects. Financing in such a manner is not sustainable, since the demand for the CTT's services is continually rising, amongst both researchers and companies (as can be seen from the results presented below).

In 2014 the Center for Technology Transfer and Innovation funded all its activities through participation in ten larger and numerous smaller EU and national projects. Projects belonged to various funding programmes and schemes: OPENiSME (CIP scheme; value 2,575,440.00 EUR), FIREMED (MED programme; value 2,407,700.00 EUR), TIPS (FP7; value 1,087,911.00 EUR), Alps4EU (Alpine Space programme; value 1,926,094.43 EUR), IP4SMEs (Cross-Border Cooperation SLO-ITA programme; value 1,350,000.00 EUR), Central Community (Central Europe programme; value 1,797,518.15 EUR), EVLIA (South-East Europe programme; value 1,455,285.00 EUR), Enterprise Europe Network Slovenia (CIP scheme; value 1,528,871.00 EUR), FIDIAS (Alpine Space programme; value 2,419,500.00 EUR), KTT (Slovenian Ministry of Economic Development and Technology; value 1,000,000.00 EUR). Project activities consisted mainly of conducting studies in the field of efficient exploitation of intellectual property rights, raising awareness on the importance of technology transfer and the protection of intangible assets, the promotion of science and applicative scientific achievements amongst companies and in society at large, the promotion of cooperation between Slovenian and international business clusters, the

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**Contract research in collaboration with industry, licensing and the formation of spin-out companies. Does the economy or researchers need them? We establish conditions, connections and facilitate.**

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**Financing through ten major and numerous smaller EU and national projects.**

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**Internally, CTT is divided into four groups, whose activities mutually interact and complement each other: GROUP for the protection and marketing of intellectual property, GROUP for contractual collaboration with economy, GROUP for promotion, education and project management, GROUP for research in the field of technology transfer and innovation.**

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development of web applications intended to support the concept of open innovation, the execution of workshops and conferences in the field of protection and marketing of intellectual property, the preparation of business plans and effective presentation of applicative innovations.

Internally, CTT is divided into four groups whose activities mutually interact and complement each other.

**Group for protection and marketing of intellectual property** deals with cases that were applied through the single entry point (44 cases), gives first advice to researchers (42), prepares assessments of patentability – reviews state of the art (30), evaluates market potential (18), helps prepare the invention for disclosure within the research organization (15), helps draft the patent application (24), prepares agreements on the ownership of intellectual property (6), chooses the patent attorney and prepares and files the patent application (24), takes care of the international (3) and national (8) expansion of patent protection. The group also prepares and passively

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**Seven license agreements with a total value of 85,500.00 EUR, 4 new companies, 29 new research topics with companies, 64 individual meetings between companies and researchers, 2 x 5 companies enabled attendance at foreign trade fairs, 20 new applications with new project partners for researchers.**

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markets technology offers (34), disseminates technology offers to specifically selected companies (7 technologies and 163 offers between September and December 2014), receives feedback and commences negotiations (19 between September and December 2014). Moreover, group members arrange for the signing of non-disclosure agreements (7), on the basis of written consent for further cooperation (8) lead negotiations (8), prepare license agreements and arranges for their signature (3 in total amount of 85,500.00 EUR). Experts that belong to this group provide individual consulting regarding all phases of spin-out company formation (13), help with the preparation of

business plans (8), manage discussions on the arrangement of the relationship between JSI and the researcher (4) and prepare license agreements for the use of technology within the company (4). To encourage the researchers in their entrepreneurship aspirations, this group's experts organize a contest for the selection of innovations with the highest commercial potential (1) and various pitching workshops for young researchers (6). Consequently, 4 new companies saw the light of day.

The above-mentioned group tightly cooperates with the **Group for contractual collaboration with economy**, which visits both large (27 since 2012) and small companies (55 in 2014), organizes their return visits to JSI (23 since 2012 as regards large companies, 3 in 2014 as regards small companies), organizes sector and regional visits of companies to JSI (2 – biotech and Danish companies) and collaborates with other support environment entities (17). This group's members are trying to find new topics for cooperation within the development projects amongst companies and researchers (75 since 2012 as regards large companies and 29 in 2014 as regards small companies), prepare technology offers (24), arrange for the signing of non-disclosure agreements (6) and acquire written consent for further cooperation (8). The group also takes part in various events; in the course of the 7<sup>th</sup> International Technology Transfer Conference it organized individual meetings between companies and researchers (64) and enabled attendance at trade fairs to groups of companies (2 x 5 companies).

**Group for promotion, education and project management** has prepared and disseminated lists of Slovenian and EU tenders (12) and foreign partner searches (1 to 8 per week, only between October and December 2014 12 contacts were successfully established), helped prepare project applications, especially in the “Exploitation” and

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**1500 visitors during the Open Day at JSI, 50 school visits and 1500 visitors throughout the year, 2 x 90 business-educated young researchers in accordance with Slovenian Research Agency's requirements, 7th International Technology Transfer Conference.**

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“Dissemination” part (4), weekly disseminated other information to TT coordinators, which has efficiently contributed to the application of new projects with foreign partners (20). The group has successfully spread various information through the monthly CTT e-newsletter and CTT's Facebook profile, organized the Open Day at JSI (1500 visitors), organized 50 school visits to JSI (with additional 1500 visitors), provided entrepreneurship education to young researchers in compliance with Slovenian Research Agency's requirements (2 x 90 visitors), organized expert excursions to companies

for young researchers (2) and organized the International Technology Transfer Conference (7th in a row). The group has successfully published new educational publications on the management of intellectual property rights and the management of project results (2).

**Group for research in the field of technology transfer and innovation** has prepared studies on the work of CTT (3), a contribution on support environment in the area of technology transfer for implementation of smart specialization procedures (1), a report on the structure of public research organizations' results according to their source and usability (1) and a study on the status of innovation activity, which served as a conclusion to the 1<sup>st</sup>

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**CTT received the “Prometej” award for excellence in communication in science for 2014.**

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National Consultation on Technology Transfer (1). The group has carried out the analysis of commercialization possibilities for EU consortia in the field of NMP (2) and ICT (1) upon European Commission's request. Upon

express invitation, the group has performed Exploitation Strategy Seminar workshops at eminent institutions, including the Fraunhofer Institute and Trinity College Dublin.

In 2014, CTT has undoubtedly reached its to-date peak, in terms of both organizational structure and results.

## INTERNATIONAL PROJECTS

1. Evaluation of Industrial Projects for Italian Partner  
Dr. Špela Stres, LLM  
Veneto Innovazione Spa
2. 7FP - TIPS; Enhancing the Capacity of EU Transport Projects to Transform Research Results into Innovative Products and Services  
Dr. Špela Stres, LLM  
European Commission
3. IPforSMEs - Intellectual Property for Small and Medium Sized Companies  
Dr. Špela Stres, LLM  
Government Office for Local Self-Government and Regional Policy
4. CE - Central Community-Emerging Communities for Collective Innovation in Central Europe  
Dr. Špela Stres, LLM  
City of Vienna, Department for EU-Strategy
5. Alps 4 EU  
Dr. Špela Stres, LLM  
European Commission
6. SEE; EVLIA - Making Full Value of Good Ideas by Leveraging Intellectual Assets for Financing SMEs in SEE  
Dr. Špela Stres, LLM  
See Programme Joint Technical Secretariat
7. MED - FireMed; Innovative Financial Instruments to Support Energy Sector SMEs in Med Area  
Dr. Špela Stres, LLM  
STC Programme MED
8. FIDIAS - Innovative Financial Instruments for Sustainable Development in Alpine Space  
Dr. Špela Stres, LLM  
European Commission
9. CIP - EACI; EASME - EIC&IRC Slovenia 1, EIC&IRC Services in Support of Business and Innovation  
Marjeta Trobec, B. Sc.  
European Commission
10. OPENiSME; Open Platform for Innovative SMEs; EACI, CIP Programme  
Dr. Špela Stres, LLM  
European Commission
11. H2020 - We4SMESLO; Enhancing the Innovation Management Capacity fo SMEs (by EEN), Slovenia  
Dr. Špela Stres, LLM  
European Commission

## R & D GRANTS AND CONTRACTS

1. IPforSMEs - Intellectual Property for Small and Medium Sized Companies  
Dr. Špela Stres, LLM
2. Technology Transfer in Public Research Institutions  
Dr. Špela Stres, LLM

## STAFF

### Researcher

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### Postdoctoral associates

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7. Urban Šegedin, B. Sc.

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10. Luka Gruden, B. Sc.
11. Lea Aissatou Kane, B. Sc.
12. France Podobnik, B. Sc.
13. Marjeta Trobec, B. Sc.
14. Luka Virag, B. Sc.

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2. A. Vorobiev, Matjaž Spreitzer, Asja Veber, Danilo Suvorov, Spartak Gevorgian, "Intrinsically tunable bulk acoustic wave resonators based on sol-gel grown PMN-PT films", *J. appl. phys.*, vol. 116, no. 6, pp. 064101-1-064101-8, 2014.

