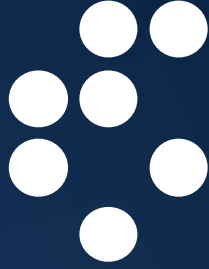
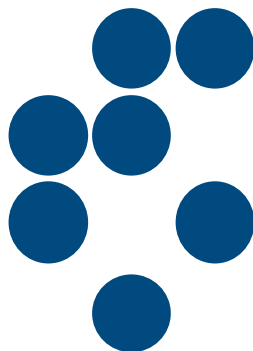


# Annual Report 2016



Jožef Stefan Institute, Ljubljana, Slovenia

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ANNUAL REPORT  
JULY 2017



# Annual Report 2016



Jožef Stefan Institute, Ljubljana, Slovenia

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# CONTENTS

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Introduction .....	5
A Brief History of the Jožef Stefan Institute .....	6
Organisation of the Jožef Stefan Institute .....	8
Management .....	10
International Advisory Board .....	10
Staff Qualifications .....	11
Recipients of the JSI awards and titles .....	12
International Cooperation .....	13
International Cooperation Agreements .....	13
Cooperation with Higher-Education Establishments .....	14
Institute Colloquia .....	17
Financing .....	18
Postgraduates Financed .....	18
Jožef Stefan Institute Undergraduate Scholarships .....	19
Completed Theses .....	20
Patents Granted .....	21
Art Exhibitions at the Jožef Stefan Institute .....	21
Awards and Appointments .....	22
Review of Publications .....	24
Knowledge Transfer .....	25
Institute in Numbers .....	26
<b>Research Departments</b>	
Department of Theoretical Physics (F-1) .....	29
Department of Low and Medium Energy Physics (F-2) .....	37
Department of Thin Films and Surfaces (F-3) .....	47
Department of Surface Engineering and Optoelectronics (F-4) .....	51
Department of Solid State Physics (F-5) .....	61
Department for Complex Matter (F-7) .....	83
Department of Reactor Physics (F-8) .....	97
Department of Experimental Particle Physics (F-9) .....	105
Department of Inorganic Chemistry and Technology (K-1) .....	115
Department of Physical and Organic Chemistry (K-3) .....	119
Electronic Ceramics Department (K-5) .....	127
Department for Nanostructured Materials (K-7) .....	135
Department for Materials Synthesis (K-8) .....	145
Department for Advanced Materials (K-9) .....	153
Department of Biochemistry, Molecular and Structural Biology (B-1) .....	159
Department of Molecular and Biomedical Sciences (B-2) .....	165
Department of Biotechnology (B-3) .....	171
Department of Environmental Sciences (O-2) .....	177
Department of Automation, Biocybernetics and Robotics (E-1) .....	193
Department of Systems and Control (E-2) .....	201
Artificial Intelligence Laboratory (E-3) .....	207
Laboratory for Open Systems and Networks (E-5) .....	213
Department of Communication Systems (E-6) .....	219
Computer Systems Department (E-7) .....	227
Department of Knowledge Technologies (E-8) .....	235
Department of Intelligent Systems (E-9) .....	245
Department of Reactor Engineering (R-4) .....	253
<b>Centres and Services</b>	
Reactor Infrastructure Centre (RIC) .....	261
Networking Infrastructure Centre (NIC) .....	265
Science Information Centre (SIC) .....	269
Energy Efficiency Centre (EEC) .....	271
Centre for Electron Microscopy and Microanalysis (CEMM) .....	275
Centre for Knowledge Transfer in Information Technologies (CT-3) .....	279
Milan Čopič Nuclear Training Centre (ICJT) .....	281
Radiation Protection Unit (SVPIS) .....	285
Centre of Technology Transfer and Innovation (CTT) .....	287



# INTRODUCTION

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

*If you don't contribute to the world's treasury of knowledge, you cannot benefit from it.*

*According to the European Commission, there is unquestionable evidence that the route to economic growth and competitiveness is strongly linked to increased investments in research and development. I find it necessary to emphasise this because it has become even clearer in the last years of the economic crisis that in spite of many declarations the differences between European countries are getting larger, with some countries, like Switzerland, Denmark, Germany, Sweden and Austria, investing heavily in research and development, while other countries are reducing investments, due to the wrong policies, or simply a lack of policies. Slovenia is, unfortunately, among those countries that do not recognise the benefits of investing in research and development, nor see them as a major opportunity for economic and social breakthroughs. The result of this indifference and political passivity is a worrying decline of the Slovenian innovation system.*

*When the public-sector austerity measures began to be introduced in Slovenia, the biggest cut was experienced by the research and development sector. Any thinking person would find it completely unreasonable to reduce the funding for research and development; there is simply no justification for such a measure. Even if Slovenes are not alone in this self-destructive behaviour, the resulting damage is immeasurable, because as a society we are losing a generation of talented people, who either go abroad or become involved in other, non-innovative activities, and are therefore lost forever to research and development. It is absurd that the greatest damage will be done to the economic sector, which is the sector of society that, in order to save on public expenditure, should be able to get the most out of it.*

*The Institute "Jožef Stefan" strives to remain as a European research centre. Every year, the share of its revenues from abroad increases, and now exceeds a quarter of its funding. Its position in Europe and our long tradition of international cooperation and exchanges are essential for the Institute and therefore we can, like every year, be proud of our excellent achievements, which find their ways into the most important scientific publications, into the sector of the economy, but also into the consciousness of the general public about the meaning of scientific research, technological development and innovations for the greater good. Inevitably our Institute leaves an important mark every year, which anyone who reads the pages of the Annual Report will recognise.*



*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



*The beginnings of robotics at the JSI, in 1985*

1987

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

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

2015

- ~ New research infrastructure, including new and renovated laboratory and office space with high-tech instrumentation for environmental research



*High-tech instrumentation for environmental research at the JSI in 2015*

## 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 Zavrtanik, 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)**

*Prof. Marko Mikuž*

### Chemistry and Biochemistry

**Inorganic Chemistry and Technology (K-1)**

*Asst. Prof. Gašper Tavčar*

**Physical and Organic Chemistry (K-3)**

*Prof. Ingrid Milošev*

**Electronic Ceramics (K-5)**

*Prof. Barbara Malič*

**Nanostructured Materials (K-7)**

*Prof. Spomenka Kobe*

**Synthesis of Materials (K-8)**

*Prof. Darko Makovec*

**Advanced Materials (K-9)**

*Prof. Danilo Suvorov*

**Biochemistry, Molecular and Structural Biology (B-1)**

*Prof. Boris Turk*

**Molecular and Biomedical Sciences (B-2)**

*Prof. Igor Križaj*

**Biotechnology (B-3)**

*Prof. Janko Kos*

**Environmental Sciences (O-2)**

*Prof. Milena Horvat*

### Electronics and Information Technology

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

*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)**

*Prof. Borka Jerman Blažič*

**Communication Systems (E-6)**

*Prof. Mihael Mohorčič*

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

*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)**  
*Dr. Igor Jenčič*

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

**Centre for Technology Transfer and Innovation (CTT)**  
*Dr. Špela Stres, MBA, LLM*

**Microanalytical Instrumental Centre (MIC)**  
*Prof. Primož Pelicon*

**Combined Atomic Microscope (UHV-AFM/STM)**  
*Prof. Maja Remškar*

**Helium Liquifier with Superconducting Magnet and Helium Regeneration System**  
*Prof. Janez Dolinšek*

**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**  
*Dr. Dušan Gabrijelčič*

## 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., Dr. Andrej Prošek*

**Workshops**  
*Franc Setnikar, B. Sc.*

## PARTICIPATION IN THE REGIONAL DEVELOPMENT OF RESEARCH

### Technology Centres

Ljubljana Technology Park Ltd.

University of Nova Gorica

Jožef Stefan International  
Postgraduate School

Technology Centre for Circuits,  
Components, Materials, Technologies and  
Equipment for Electrotechnic (TC SEMTO)

Nanotesla Institute Ljubljana

Development Centre for Hydrogen  
Technologies

Technology Centre for Production  
Automation, Robotics and Informatics  
(ARI)

Security Technology  
Competence Centre (SETTCE)

### Centres of Excellence

Nanocenter - Center of Excellence in  
Nanoscience and Nanotechnology

Centre of Excellence for Integrated  
Approaches in Chemistry and Biology  
of Proteins (CIPKeBiP)

Centre of Excellence NAMASTE

Centre of Excellence for Polymer  
Materials and Technologies (PoliMaT)

EN-FIST Centre of Excellence

CEBIC Centre of Excellence for Biosensors,  
Instrumentation and Process Control

CO NOT: Centre of Excellence for Low-  
Carbon Technologies

Centre of Excellence for Space Sciences  
and Technologies SPACE-SI

# MANAGEMENT

---

## DIRECTORATE

### Director JSI

Prof. Jadran Lenarčič

### Assistant to the Director

Dr. Romana Jordan

### Adviser

Marta Slokan, LL. B.

## BOARD OF GOVERNORS

Dr. Mark Pleško, *Chair, Cosylab, d. d., Ljubljana*

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

Prof. Marko Mikuž, *JSI*

Stojan Petrič, *Kolektor, d. o. o., Idrija*

Prof. Jože Pungerčar, *JSI*

Dr. Iztok Seljak, *Hidria, d. o. o., Ljubljana*

Prof. Stanko Strmčnik, *JSI*

Mrs. Kim Turk, *Ministry of Education, Science and Sport*

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

## SCIENTIFIC COUNCIL

Prof. Dragan Dragoljub Mihailovič, *President*

Prof. Leon Cizelj

Prof. Miran Čeh

Prof. Milena Horvat

Prof. Đani Juričič

Prof. Spomenka Kobe

Prof. Jadran Lenarčič

Prof. Marko Mikuž

Prof. Ingrid Milošev, *Deputy President*

Prof. Dunja Mladenčić, *Deputy President*

Prof. Franc Novak

Prof. Peter Prelovšek

Prof. Maja Remškar

Prof. Žiga Šmit

Prof. Boris Turk

# 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

Prof. John H. Beynon, University of Wales Swansea, Swansea, United Kingdom

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

Prof. Bernard Roth, Stanford University, Stanford, California, USA

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

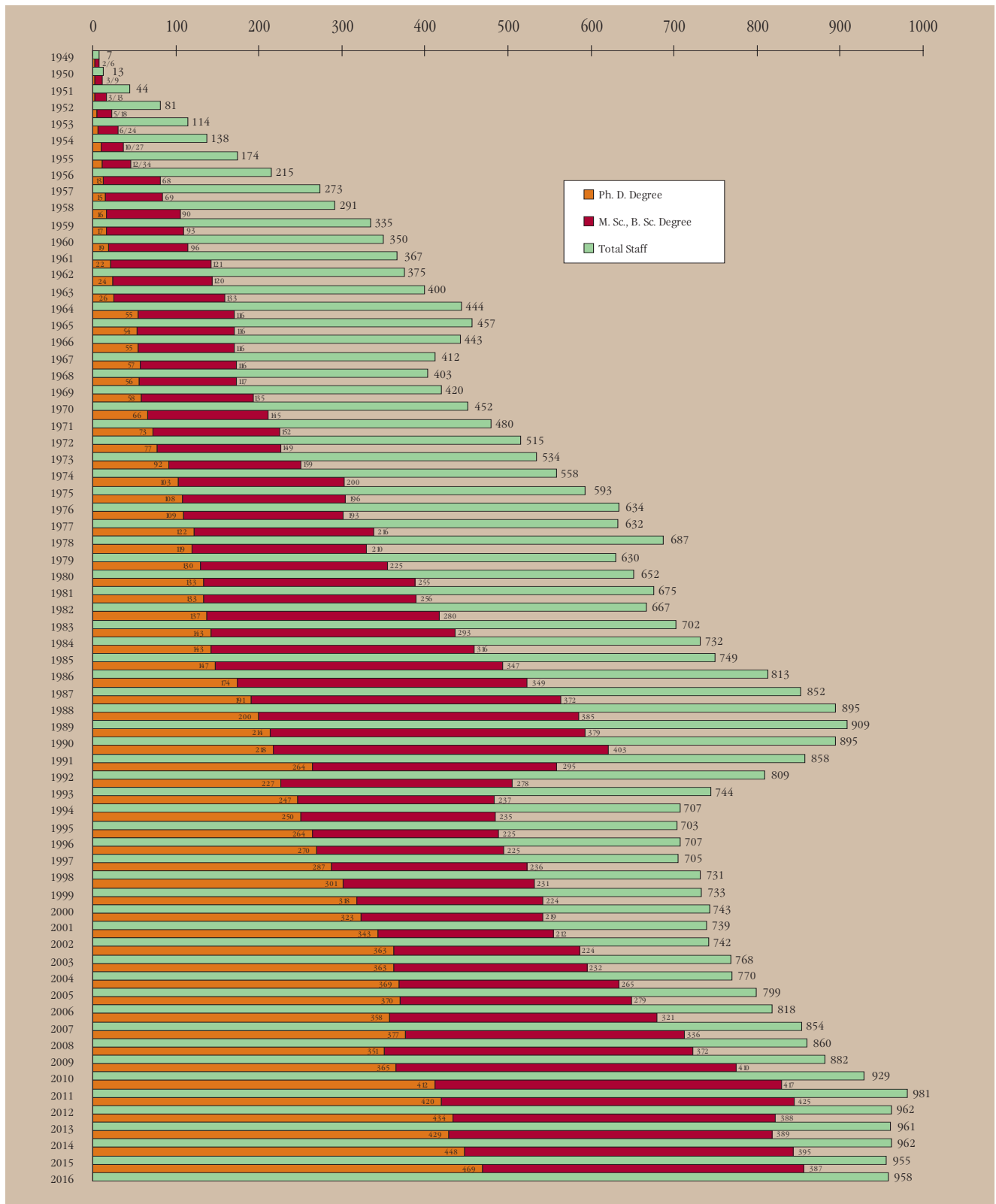
Prof. Volker Sörgel, Ruprecht-Karis-Universität, Heidelberg, Germany

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

Prof. Thomas Walcher, Universität Mainz, Mainz, Germany

# STAFF QUALIFICATIONS

1949-2016



# RECIPIENTS OF THE JSI AWARDS AND TITLES

## HONORARY MEMBERS

- Prof. Robert Blinc<sup>☞</sup>, President of the Scientific Council of the Jožef Stefan Institute from 1992 to 2007 (1933 - 2011)
- Prof. Jean-Marie Dubois, Institut Jean Lamour, CNRS - Centre National de la Recherche Scientifique, Paris and Université Lorraine, Nancy, France
- Prof. Boris Frlec, Director of the Jožef Stefan Institute from 1975 to 1984
- Prof. Robert Huber, Nobel Prize Winner, Max-Planck-Institut für Biochemie, Munich, Germany
- Prof. Milan Osredkar<sup>☞</sup>, Director of the Jožef Stefan Institute from 1963 to 1975 (1919 - 2003)
- Prof. Anton Peterlin<sup>☞</sup>, Founder and First Director of the Jožef Stefan Institute from 1949 to 1955 (1908 - 1993)

## ASSOCIATE MEMBERS

- Prof. David C. Ailion, University of Utah, Salt Lake City, Utah, USA
- Prof. Neil Bartlett<sup>☞</sup>, University of California, Berkeley, California, USA
- Prof. John H. Beynon, University of Wales Swansea, Swansea, United Kingdom
- Prof. Wolfram Bode, Max-Planck-Institut für Biochemie, Munich, Germany
- Prof. Oscar D. Bonner<sup>☞</sup>, University of South Carolina, Columbia, South Carolina, USA
- Dr. Horst Borrmann, Max-Planck-Institut für chemische Physik fester Stoffe, Dresden, Germany
- Prof. Henrik Buchowsky, Politechnika Warszawska, Warszawa, Poland
- Prof. Rüdiger Dillmann, Karlsruher Institut für Technologie, Karlsruhe, Germany
- Prof. Joseph W. Doane, Liquid Crystal Institute, Kent State University, Kent, Ohio, USA
- Prof. Hans Fritz, Universität München, Munich, Germany
- Prof. Oskar Glemser<sup>☞</sup>, Universität Göttingen, Göttingen, Germany
- Prof. Paul Hagenmuller, Université de Bordeaux I, Bordeaux, France
- Prof. John Holloway, University of Leicester, Leicester, United Kingdom
- Prof. Rudolf Hoppe<sup>☞</sup>, Universität Giessen, Giessen, Germany
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- Prof. Nobuhiko Katunuma, Tokushima Bunri University, Tokushima, Japan
- Prof. Raymond Kind, ETH, Zurich, Switzerland
- Prof. Jože Koller, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia
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- Dr. Fani Milia, National Centre for Scientific Research "Demokritos", Athens, Greece
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- Prof. Vincenzo Parenti - Castelli, University of Bologna, Bologna, Italy
- Prof. Herbert W. Roesky, Universität Göttingen, Göttingen, Germany

- Prof. John A. Rupley, The University of Arizona, Tucson, Arizona, USA
- Prof. Findlay E. Russell, The University of Arizona, Tucson, Arizona, USA
- Prof. Hugo V. Schmidt, Montana State University, Bozeman, Montana, USA
- Prof. Lev A. Shuvalov<sup>☞</sup>, Institute for Crystallography, Russian Academy of Sciences, Moscow, Russia
- Prof. Neil W. Tanner<sup>☞</sup>, University of Oxford, Oxford, United Kingdom
- Dr. Alain Tressaud, Institut de Chimie de la Matière Condensée de Bordeaux, CNRS, Pessac, France
- Prof. Vlado Valković, Zagreb, Croatia
- Prof. John Waugh, M.I.T., Cambridge, Massachusetts, USA

## EMERITUS SCIENTISTS

- Prof. France Bremšak<sup>☞</sup>
- Prof. Mihael Drofenik
- Prof. Peter Gosar
- Prof. Darko Jamnik
- Prof. Gabrijel Kernel
- Prof. Borut Mavko
- Prof. Miodrag V. Mihailović<sup>☞</sup>
- Prof. Raša Matija Pirc
- Prof. Marjan Senegačnik<sup>☞</sup>
- Prof. Saša Svetina
- Prof. Boštjan Žekš
- Prof. Boris Žemva

## EXTERNAL ADVISERS

- Prof. Savo Bratoš, Université Pierre et Marie Curie, Paris, France
- Marko Bulc, B. Sc., Ljubljana, Slovenia
- Prof. Davorin Dolar<sup>☞</sup>, Slovenian Academy of Sciences and Arts, Ljubljana, Slovenia
- Zdravko Gabrovšek, B. Sc., Slovenia
- Prof. Dušan Hadži, National Institute of Chemistry, Ljubljana, Slovenia
- Prof. Karl A. Müller, *Nobel Prize Winner*, IBM Research Laboratory, Zurich, Switzerland
- Prof. Bogdan Povh, Max-Planck-Institut für Kernphysik, Heidelberg, Germany
- Dr. Lev Premrú<sup>☞</sup>, Lek, d. d., Ljubljana, Slovenia
- Prof. Momčilo M. Ristić, Academy of Science of Serbia, Belgrade, Serbia
- 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 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)	74
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	64
ESRR	12
OTHERS (COST, IAEA, IEE, JRC, IRMM, ESA, NATO, CIP, MED, EMRP, EMPIR, WHO, LIFE+, SCOPES...)	154
<b>TOTAL</b>	<b>304</b>

Bilateral cooperation	No. of projects
Argentina	1
Austria	2
Montenegro	2
France	14
Croatia	8
India	3
Japan	3

Bilateral cooperation	No. of projects
Russia	5
Serbia	10
Turkey	3
USA	27
Bosnia and Herzegovina	2
Others	7
<b>TOTAL</b>	<b>87</b>

## In 2016, international cooperation agreements were signed between the Jožef Stefan Institute and:

1. UChicago Argonne, LLC, Argonne National Laboratory, Argonne, IL, USA (F2, F7)
2. TUNAP Industrie Chemie GmbH & Co Produktions KG, Wolfratshausen, Germany (F5, CTT)
3. DIC Corporation, Tokyo, Japan (F5)
4. Innovidis AB, Gothenburg, Sweden (F5)
5. CEA - Commissariat a l'Energie Atomique et aux Energies Alternatives, Paris, France (F8)
6. Joint Research Centre of the European Commission, Directorate for Health, Consumers and Reference Centre, Geel, Belgium; Bor Kos, Jesenice, Slovenia (F8)
7. Ulsan National Institute of Science and Technology, School of Mechanical and Nuclear Engineering, Ulsan, Republic of Korea (F8)
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17. South China University of Technology, Department of Electronic Materials Science and Engineering, Guangzhou, P.R. China (K9)
18. Centro de Desenvolvimento da Tecnologia Nuclear - CDTN, Belo Horizonte - Minas Gerais, Brazil (O2)
19. Masaryk University, Faculty of Science, Research Centre for Toxic Compounds in the Environment (RECETOX), Brno, Czech Republic (O2)
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28. Donders Institute for Brain, Cognition and Behaviour, Centre for Cognitive Neuroimaging, Nijmegen, The Netherlands (E7, CTT)
29. Czech Technical University in Prague, Prague 6, Czech Republic (E8)
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31. Shanghai Jiao Tong University, School of Nuclear Science and Engineering, ICB for Basic Research on Thermal-Hydraulic of Advanced Nuclear Reactor System, Shanghai, P.R.China (R4)
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### Assistants and researchers

1. Asst. Prof. Marko Bračko, University of Maribor, Faculty of Chemistry and Chemical Engineering
2. Dr. Jure Leskovec, Stanford University, Palo Alto, California, USA
3. Dr. Tomaž Rejec, University of Ljubljana, Faculty of Mathematics and Physics
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36. Asst. Prof. Robert Jeraj, University of Ljubljana, Faculty of Mathematics and Physics, University of Wisconsin, School of Medical Physics, Madison
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41. Prof. Monika Kapus Kolar, University of Maribor, Faculty of Electrical Engineering and Computer Science
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53. Asst. Prof. Dušan Kordiš, University of Ljubljana, Biotechnical Faculty, Faculty of Chemistry and Chemical Technology, IPS, Ljubljana
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57. Dr. Igor Kovač, Fachhochschule Joaneum, Graz, Austria
58. Asst. Prof. Janez Kovač, University of Ljubljana, Faculty of Natural Sciences and Technology and IPS, Ljubljana
59. Prof. Igor Križaj, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Biotechnical Faculty, Medical Faculty, IPS, Ljubljana
60. Asst. Prof. Danjela Kuščer Hrovatin, IPS, Ljubljana
61. Prof. Zdravko Kutnjak, University of Ljubljana, Faculty of Mathematics and Physics and Faculty of Mechanical Engineering, IPS, Ljubljana
62. Prof. Nada Lavrač, University of Nova Gorica, IPS, Ljubljana, University of Ljubljana
63. Prof. Jadran Lenarčič, University of Ljubljana, Faculty of Electrical Engineering, University of Nova Gorica, Università degli studi di Bologna
64. Asst. Prof. Igor Lengar, University of Maribor, Faculty of Energy Technology
65. Asst. Prof. Matej Lipoglavšek, University of Ljubljana, Faculty of Mathematics and Physics
66. Asst. Prof. Darja Lisjak, IPS, Ljubljana
67. Prof. Sonja Lojen, University of Nova Gorica, School of Environmental Sciences
68. Prof. Boris Majaron, University of Ljubljana, Faculty of Mathematics and Physics
69. Prof. Darko Makovec, University of Maribor, Faculty of Chemistry and Chemical Engineering and Faculty of Medicine, IPS, Ljubljana
70. Prof. Barbara Malič, IPS, Ljubljana
71. Asst. Prof. Igor Mandič, University of Ljubljana, Faculty of Natural Sciences and Technology
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75. Asst. Prof. Tomaž Mertelj, University of Ljubljana, Faculty of Mathematics and Physics
76. Prof. Dragan Dragoljub Mihailović, University of Ljubljana, Faculty of Mathematics and Physics and IPS, Ljubljana
77. Asst. Prof. Andrej Mihelič, University of Ljubljana, Faculty of Mathematics and Physics
78. Prof. Radmila Milačič, IPS, Ljubljana
79. Prof. Ingrid Milošev, University of Zagreb, Croatia, Faculty of Chemical Engineering and Technology and IPS, Ljubljana
80. Prof. Dunja Mladenič, IPS, Ljubljana and University of Zagreb, Croatia, University of Ljubljana, Faculty of Education, University of Nova Gorica, University of Primorska, Koper
81. Asst. Prof. Mihael Mohorčič, IPS, Ljubljana
82. Prof. Miran Mozetič, University of Nova Gorica, IPS, Ljubljana, University of Ljubljana, Faculty of Natural Sciences and Technology
83. Asst. Prof. Bojan Nemeč, IPS, Ljubljana
84. Prof. Franc Novak, University of Maribor, Faculty of Electrical Engineering and Computer Science and IPS, Ljubljana



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89. Asst. Prof. Primož Pelicon, University of Ljubljana, Faculty of Mathematics and Physics
90. Asst. Prof. Toni Petan, University of Ljubljana, Biotechnical Faculty, Faculty of Chemistry and Chemical Technology, IPS, Ljubljana
91. Asst. Prof. Maja Ponikvar-Svet, IPS, Ljubljana
92. Prof. Jože Pungercar, University of Ljubljana, Biotechnical Faculty, Faculty of Chemistry and Chemical Technology, IPS, Ljubljana
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98. Prof. Borut Smodiš, University of Ljubljana, Faculty of Chemistry and Chemical Technology, University of Nova Gorica, School of Environmental Sciences and IPS, Ljubljana
99. Asst. Prof. Luka Snoj, University of Ljubljana, Faculty of Mathematics and Physics
100. Asst. Prof. Matjaž Spreitzer, University of Ljubljana, Faculty of Chemistry and Chemical Technology
101. Prof. Marko Starič, University of Ljubljana, Faculty of Mathematics and Physics
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107. Prof. Janez Ščančar, IPS, Ljubljana
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110. Asst. Prof. Miha Škarabot, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Mathematics and Physics
111. Asst. Prof. Primož Škraba, University of Nova Gorica, Center for Atmospheric Research and University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies
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113. Asst. Prof. Janez Štrancar, IPS, Ljubljana
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115. Asst. Prof. Aleš Švigelj, IPS, Ljubljana
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119. Asst. Prof. Roman Trobec, University of Ljubljana, Faculty of Computer and Information Science
120. Prof. Boris Turk, University of Ljubljana, Biotechnical Faculty, Faculty of Chemistry and Chemical Technology, IPS, Ljubljana
121. Prof. Dušan Turk, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Medicine, IPS, Ljubljana
122. Prof. Vito Turk, University of Ljubljana, Faculty of Chemistry and Chemical Technology, IPS, Ljubljana
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138. Asst. Prof. Kristina Žužek Rožman, IPS, Ljubljana

### Assistants and researchers

1. Dr. Tanja Arh, IPS, Ljubljana, DOBA Faculty of Applied Business and Social Studies, Maribor
2. Dr. Zoran Arsov, University of Ljubljana, Faculty of Mathematics and Physics
3. Dr. Samir El Shawish, University of Ljubljana, Faculty of Mathematics and Physics
4. Dr. Blaž Fortuna, IPS, Ljubljana
5. Matej Gašperin, B. Sc., University of Nova Gorica
6. Dr. Dejan Gradišar, University of Ljubljana, Faculty of Electrical Engineering
7. Dr. Andrej Hrovat, IPS, Ljubljana
8. Dr. Peter Jeglič, University of Ljubljana, Faculty of Mathematics and Physics
9. Dr. Boštjan Kaluža, IPS, Ljubljana
10. Dr. Martin Klanjšek, University of Ljubljana, Faculty of Mathematics and Physics
11. Dr. Andraž Kocjan, IPS, Ljubljana
12. Dr. Boštjan Končar, University of Ljubljana, Faculty of Mathematics and Physics
13. Dr. Petra Kralj Novak, IPS, Ljubljana
14. Dr. Marjan Kromar, University of Maribor, Faculty of Energy Technology
15. Dr. Matjaž Leskovar, University of Ljubljana, Faculty of Mathematics and Physics
16. Dr. Mitja Luštrek, IPS, Ljubljana
17. Dr. Matija Milanič, University of Ljubljana, Faculty of Mathematics and Physics
18. Dr. Natan Osterman, University of Ljubljana, Faculty of Mathematics and Physics
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23. Dr. Špela Stres, University of Ljubljana, Faculty of Electrical Engineering
24. Dr. Andrej Studen, University of Ljubljana, Faculty of Mathematics and Physics
25. Tina Šfiligoj, B. Sc., University of Ljubljana, Faculty of Mathematics and Physics
26. Tea Tušar, M. Sc., IPS, Ljubljana
27. Dr. Mitja Uršič, University of Ljubljana, Faculty of Mathematics and Physics
28. Dr. Mojca Vilfan, University of Ljubljana, Faculty of Mathematics and Physics
29. Dr. Andrija Volkanovski, University of Ljubljana, Faculty of Mathematics and Physics
30. Dr. Darko Vrečko, University of Nova Gorica, School of Environmental Sciences
31. Dr. Andrej Zorko, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Mathematics and Physics
32. Dr. Gašper Žerovnik, University of Ljubljana, Faculty of Mathematics and Physics

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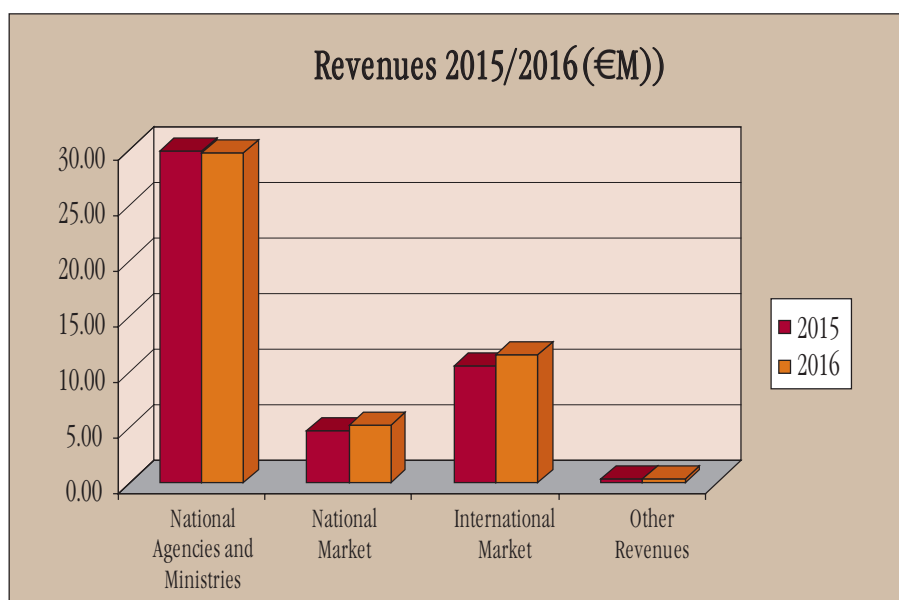
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# FINANCING

## REVENUES JSI (€) AND NUMBER OF PROJECTS

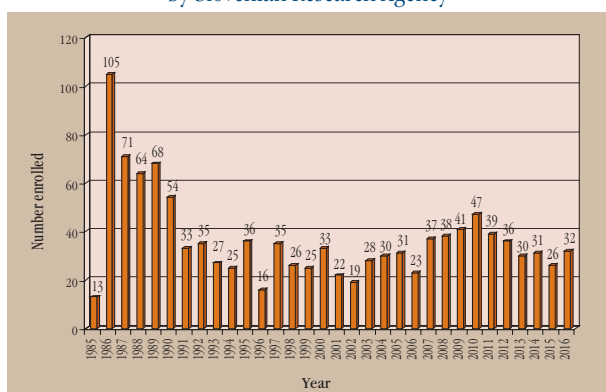
	Contribution		Contribution		Index 2016/2015	No. of Projects in 2016
	2016	2016	2015	2015		
National Agencies and Ministries	29,844,964	63.4 %	29,980,897	65.8 %	99.5	398
National Market	5,244,775	11.1 %	4,703,687	10.3 %	111.5	223
International Market	11,645,413	24.7 %	10,535,749	23.1 %	110.5	328
Other Revenues	340,525	0.7 %	358,872	0.8 %	94.9	
<b>TOTAL</b>	<b>47,075,677</b>	<b>100.0 %</b>	<b>45,579,205</b>	<b>100.0 %</b>	<b>103.3</b>	<b>949</b>



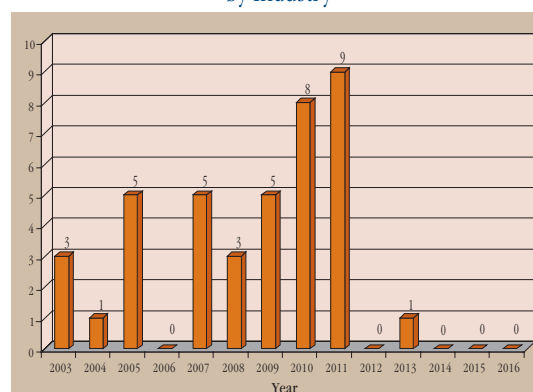
## POSTGRADUATES FINANCED

1985-2016

by Slovenian Research Agency



by Industry



# JSI UNDERGRADUATE SCHOLARSHIPS

1977-2016

Year	FMF		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
2015	21	6	4		1				9	1			10	52
2016	16	2	5						7	1			15	46
<b>TOTAL</b>	<b>437</b>	<b>106</b>	<b>434</b>	<b>25</b>	<b>13</b>	<b>8</b>	<b>4</b>	<b>63</b>	<b>479</b>	<b>33</b>	<b>20</b>	<b>11</b>	<b>48</b>	<b>1681</b>

**FMF** 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

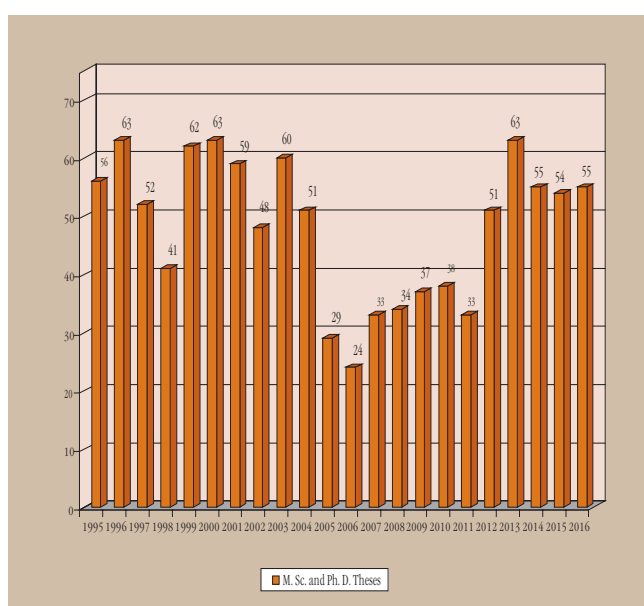
**FE** Faculty of Electrical Engineering, University of Ljubljana  
**FRI** Faculty of Computer and Information Science, University of Ljubljana  
**FG** Faculty of Civil Engineering, University of Maribor  
**FERI** Faculty of Electrical Engineering and Computer Science, University of Maribor  
**UNG** 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 2016

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
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

Year	Ph. D. Theses	M. Sc. Theses	Total
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
2015	44	10	54
2016	42	13	55
<b>TOTAL</b>	<b>1125</b>	<b>881</b>	<b>2006</b>



# PATENTS GRANTED

1. Alenka Vesel, Miran Mozetič, Rok Zaplotnik  
Device for high-frequency gas plasma excitation  
DE112012000015 (B4), Deutsches Patent- und Markenamt, 21. 04. 2016.
2. Matjaž Lukač, Zdenko Vižintin, Boris Cenčič  
Method for lightening or eradicating pigments in human skin  
US9254174 (B2), US Patent Office, 09. 02. 2016.
3. Igor Muševič, Matjaž Humar  
Spherical liquid-crystal laser  
US9263843 (B2), US Patent Office, 16. 02. 2016.
4. P. E. Galavis, Bhudatt R. Paliwal, James E. Holden, Robert Jeraj  
System and method for gradient assisted non-connected automatic region (GANAR) analysis  
US9355447 (B2), US Patent and Trademark Office, 31. 05. 2016.
5. Janko Petrovčič, Damir Vrančič  
Reducing oscillations in a control system  
EP2356522 (B1), European Patent Office, 06. 01. 2016.
6. Rok Zupet, Jernej Iskra, Miloš Ružič, Anica Pečavar, Ivanka Kolenc, Jože Pucelj, Igor Plaper  
A process for a preparation of marbofloxacin and intermediate thereof  
EP2501680 (B1), European Patent Office, 10. 02. 2016.
7. Xinzhen Zhang, Jingjun Xu, Wei Li, Irena Drevenšek Olenik, Wei Cui, Bin Shi, Zhenhua Wang, Qiang Wu, Yongfa Kong  
Micro/nano region liquid crystal alignment method and system thereof based on laser direct writing  
CN103995394 (B), Chinese Patent Office, 17. 08. 2016.
8. Igor Vaskivskiy, Dragan Mihailović, Ian Mihailović  
Switchable macroscopic quantum state devices and methods for their operation  
SI24776 (A), Slovenian Intellectual Property Office, 29. 01. 2016.
9. Gregor Papa, Barbara Koroušič-Seljak, Marko Pavlin  
Device and method for acquisition and transfer of signals  
SI24792 (A), Slovenian Intellectual Property Office, 29. 02. 2016.
10. Matjaž Gams, Hristijan Gjoreski, Mitja Luštrek  
Method and system for detecting a person driving a vehicle while using a mobile computing device  
SI24796 (A), Slovenian Intellectual Property Office, 29. 02. 2016.
11. Luka Suhadolnik, Matic Krivec, Miran Čeh, Kristina Žagar, Goran Dražič  
Photocatalytic reactor  
SI24802 (A), Slovenian Intellectual Property Office, 31. 03. 2016.
12. Matjaž Vencelj, Larisa Hosnar, Klemen Bučar, Janez Burger  
Angle-sensitive gamma camera with a rotary obstruction  
SI24818 (A), Slovenian Intellectual Property Office, 31. 03. 2016.
13. Alenka Vesel, Rok Zaplotnik, Miran Mozetič  
Method for cleaning of with body fluid-contaminated medical implantants and devices with the use of atomic oxygen  
SI24840 (A), Slovenian Intellectual Property Office, 29. 04. 2016.
14. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič  
A method of colouring titanium and titanium alloys  
SI24851 (A), Slovenian Intellectual Property Office, 29. 04. 2016.
15. Matjaž Vencelj, Miha Cankar, Andrej Likar  
Process and device for improvement of operation of silicon photomultipliers in the regime of piled-up pulses of light  
SI24863 (A), Slovenian Intellectual Property Office, 29. 04. 2016.
16. Aleš Lapanje  
The impregnation process and attachment of microorganisms in porous materials  
SI24910 (A), Slovenian Intellectual Property Office, 29. 07. 2016.
17. Andrej Kovič, Adolf Jesih, Aleš Mrzel  
Process for the synthesis of the molybdenum carbide in the form of quasi-one-dimensional structures, that is, nano-wires, micro-wires, nano-strips and micro-strips  
SI24925 (A), Slovenian Intellectual Property Office, 31. 08. 2016.
18. Tadej Rejc, Uroš Petrič, Jana Debeljak, Toni Bremec, Polonca Ferik, Mojca Lunder, Irena Roškar, Borut Štrukelj, Samo Kreft  
Mixture of natural polyphenols from white fir wood for reducing postprandial glucose concentration  
SI24984 (A), Slovenian Intellectual Property Office, 30. 11. 2016.
19. Peter Dušak, Marin Berovič, Darko Makovec  
Process for regulation of lactic acid fermentation in wine production by magnetic elimination of bacteria  
SI24998 (A), Slovenian Intellectual Property Office, 30. 11. 2016.

# ART EXHIBITIONS AT THE JSI

Suzi Bricej, 25 January-18 February  
 Evgenija Jarc and Andrej Mivšek, 22 February-17 March  
 Andrej Jemec, 21 March-21 April  
 Janez Kukec Mezek, 25 April-18 May  
 Teo Spiller, 23 May-15 June  
 Istvan Išt Huzjan, 31 May (Forma Viva)  
 Vesna Drnovšek, 20 June-11 July  
 Denise Eyer-Oggier, 11 July-1 September  
 Lucija Stramec, 5 September-6 October  
 Milan Razboršek, 10 October-3 November  
 Mito Gegič, 7 November-8 December  
 Zoran Ogrinc, 12 December-13 January 2017



*Acedemician Prof. Andrej Jemec at the opening of his exhibition*

# AWARDS AND APPOINTMENTS

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

### Zois Certificate of Recognition

**Jernej Fescl Kamenik**

Presented with the Zois Certificate of Recognition for the search for new physics in the theory of elementary particles



*The winner of Zois Certificate of Recognition: Asst. Prof. Jernej Fescl Kamenik*

## JSI AWARDS AND APPOINTMENTS

### The Jožef Stefan Golden Emblem Prize

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

**Ljupka Stojčevska Malbašič**

Femtosecond relaxation dynamics in collective-electronic-state materials: cuprate and iron pnictide superconductors and charge-density wave systems

**Miha Grilc**

Kinetics of the liquefaction process and catalytic deoxygenation of lignocellulosic biomass

**Dejan Dovžan**

Recursive fuzzy identification in control and process monitoring

### The Jožef Stefan Roll of Honour

was awarded for their successful contribution for developing new high-tech products based on scientific and technological achievements of the Jožef Stefan Institute:

**Dr. Janez Pirš**

**Janez Škrlec**

## OTHER SELECTED AWARDS TO JSI RESEARCHERS

**Department of Knowledge Technologies (JSI)**, Special Recognition for Successful Cooperation with the Committee on Science and Technology of the Chamber of Craft and Small Business of Slovenia and for an interesting presentation of the Department of Knowledge Technologies of the Jožef Stefan Institute at the International Fair of Crafts and Entrepreneurship in Celje.

**Energy Efficiency Centre (JSI)**, Award TARAS – for successfully carrying out the project for the useful exploitation of waste heat in the steel industry in the district heat system in Ravne na Koroškem, which is a recognition for the most successful cooperation of economy and scientific research work

**Darko Belavič**, Elected to the serving member of Electrotechnical Association Slovenia, MIDEM – Proposer: Society for Microelectronics, Electronic Components and Materials, Ljubljana, Slovenia May, 2016

**Blaž Belec**, 3<sup>rd</sup> award for presentation at the 8. Conference of Jožef Stefan International Postgraduate School, Ljubljana, Jožef Stefan International Postgraduate School.

**Blaž Belec**, Best contribution at the 8. Conference of Jožef Stefan International Postgraduate School, Ljubljana, Jožef Stefan International Postgraduate School.

**Janez Bonča**, Article in Nature Physics entitled: Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates, was selected as one of the most excellent scientific achievements in science in the year 2015.

**Andraž Bradeško**, Best poster award, Institute of Electrical and Electronics Engineers (IEEE), ISAF/ECAPD/PFM Conference 2016 – IEEE, Darmstadt, Germany, August 21-25, 2016



*The winners of the Jožef Stefan Golden Emblem Prize: Dr. Ljupka Stojčevska Malbašič, Dr. Miha Grilc and Dr. Dejan Dovžan*

**Martin Breskvar, Dragi Kocev, Jurica Levatič, Aljaž Osojnik, Matej Petkovič, Nikola Simidjievski and Bernard Ženko** won the ESA's Mars Express Power Challenge, designing the most accurate solution for predicting a space probe's power consumption.

**Primož Cigoj**, The Second best Innovation: "MUPOSS" product, 9th International Technology Transfer Conference, Brdo pri Kranju, Slovenia, September 21 2016

**Oriol Costa Garrido**, Winner prize for the best presentation of relevant research in nuclear fields (ENC 2016 conference, Warsaw, Poland), European Nuclear Education Network, Life-time predictions accuracy of the thermally fatigued pipes under turbulently mixing fluids

**Oriol Costa Garrido**, Best poster award (ICONE 24 conference, Charlotte, North Carolina, USA), American Society of Mechanical Engineers, Probabilistic prediction of fatigue life of pipes under turbulent fluid mixing

**Sašo Džeroski**, corresponding member of the Macedonian Academy of Arts and Sciences, was elected for a full member of the European Academy of Sciences (Academia Europaea).

**Lovro Fulanovič**, SHAPING VI, Student poster award winner, Montpellier, France, July 20, 2016



*The winners of the Jožef Stefan Roll of Honour, for their successful contribution to developing new, high-tech products based on the scientific and technological achievements of the Jožef Stefan Institute: Janez Škrlec & Prof. Barbara Malič (left) and Dr. Janez Pirs (right)*

**Urška Gabor**, Award for best oral presentation in young researchers section at the 24th International Conference on Materials and Technology, Portorož, Metals and Technology (IMT), "Different approaches to avoiding lead deficiency in PMN-PT thin films"

**Ana Gantar, Nataša Drnovšek, Rok Kocen, Saša Novak**, Special prize for Innovations for Economy for "SilkPatch - Innovative Solution for Chronic Skin Wounds", 9th International Technology Transfer Conference & Innovation Day 2016, Brdo pri Kranju, 21 September 2016

**Tanja Goršak**, Best presentation at the 8. Conference of Jožef Stefan International Postgraduate School, Ljubljana, Jožef Stefan International Postgraduate School.

**Tadej Holler**, Best paper award (ICONE 24 conference, Charlotte, North Carolina, USA), American Society of Mechanical Engineers, Large-scale homogeneous hydrogen-air-steam deflagration experiment simulated using two turbulent flame speed closure models

**Matjaž Humar**, 1<sup>st</sup> Place Poster Prize at prestigious Nobel Laureate Meeting 2016, Lindau, Germany. Matjaž presented a poster about lasers embedded into single live cells for the first time. He has also demonstrated that fat cells already present in human body already contain tiny lasers, which only need to be activated.

**Tanja Kaiba**, Prešeren Award, Ljubljana, Slovenia, 6. 12. 2016, Faculty of Mathematics and Physics, University of Ljubljana, for the master thesis entitled: Fission and ionization chambers response at the JSI TRIGA reactor

**Janez Kokalj, Matjaž Leskovar, Mitja Uršič**, Best poster award (NENE 2016 conference, Portorož, Slovenia), Nuclear Society of Slovenia, Modelling of Debris Bed Coollability in Bottom Reflooding Conditions with MC3D

**Bor Kos**, Young author award. Young author award committee at the international conference NENE 2016, Portorož, 5.-8. 9. 2016, for the contribution entitled "Variance Reduction of Fusion and Fission Neutron Transport Problems using the ADVANTG Hybrid Code" co-authored by Ivan A. Kodeli

**Tomaž Kos**, The 2016 Prešeren award at the University of Ljubljana, Faculty of Electrical Engineering for his research project entitled Measurement system for automated low-frequency and high-temperature characterization of dielectric materials

**Tomaž Kos**, Tadej Rojac (co-mentor), Prešeren Award, Faculty of Electrical Engineering, Ljubljana, Slovenia, December 6, 2016

**Nina Kostevšek**, Best Young Lecturer Award, 2nd International Symposium on Nanoparticles-Nanomaterials and Applications (ISN2A-2016), Lisbon, Portugal, 8-21 January 2016. Title of the awarded contribution: "Multimodal hybrid FePt/SiO<sub>2</sub>/Au nanoparticles for nanomedical applications: New synthesis approach for improved magnetic and optical properties" (co-authors: Sašo Šturm, Igor Serša, Ana Sepe, Matjaž Spreitzer, Spomenka Kobe, Kristina Žužek Rožman)

**Matic Kunšek**, Certificate; European master of nuclear engineering (IAEA General Conference, Vienna, Austria), European Nuclear Education Network

**Danjela Kuščer, Janez Holc and from ETI d.d.: Ines Bantan, Joži Prašnikar, Helena Razpotnik**, Silver Award for innovation: "Neporočni kordieritni material C410 za elektrotehniko", Gospodarska zbornica Slovenije, Zasavje, Slovenia, June 8, 2016

**Matej Petkovič** was awarded the Prešeren Prize of the Faculty of Mathematics and Physics of the University of Ljubljana for his Master's thesis titled "Evaluation of the importance of continuous features with the Relief method", written under supervision of Sašo Džeroski.

**Rudolf Podgornik**, "Sackler Scholar", Israel, Mortimer and Raymond Sackler Institute of Advanced Studies, Tel Aviv University in the academic year 2016/2017, selected for "eminence in his field of research".

**Vid Podpečan** received the Prometheus of Science award for excellence in communication for the year 2016 by the Slovenian Science Foundation for all-round promotion of robotics, especially humanoid robot use among young people.

**Luka Snoj**, Name of the Month on the Radio Val 202, June 2016, Ljubljana, Slovenia, awarded by RTV Slovenia, Radio Val 202

**Stanislav Strmčnik**, received the Professor Emeritus of the University of Nova Gorica award for his significant contribution to the development of scientific activities and his remarkable performance as professor and mentor

**Luka Suhadolnik**, 3<sup>rd</sup> Best Oral Presentation at the 24th International Conference on Materials and Technology, Portorož, Slovenia, 28-30 September 2016. Title of the awarded contribution: Optimization of Photoelectrocatalytic Activity of TiO<sub>2</sub>-based Microreactor (co-authors: Andrej Pohar, Blaž Likožar and Miran Čeh)

**Martin Štefanič**, Seal of Excellence, Brussels, Belgium, European Commission, project proposal NanoDryCell: Nanoparticle-assisted desiccation of mesenchymal stem cells for the "off-the-shelf" allogeneic cell therapy

**Aleš Švigelj, Kemal Alič, Radovan Srnc**, the Best Paper Award of the IEEE ComSoc Technical Committee on Communications Systems Integration and Modeling, "Network traffic modeling for load prediction: a user-centric approach", IEEE Network, IEEE Globecom 2016, Washington, USA, December 2016.



# REVIEW OF PUBLICATIONS

FOR 2016

Department	Original Articles*	Books	Patent Appl. and Grants	Theses
Department of Theoretical Physics (F-1)	99	1		3
Department of Low and Medium Energy Physics (F-2)	79	2	2	2
Department of Thin Films and Surfaces (F-3)	21			
Department of Surface Engineering and Optoelectronics (F-4)	58		3	
Department of Solid State Physics (F-5)	118	7	3	5
Department for Complex Matter (F-7)	47		4	5
Department of Reactor Physics (F-8)	69	2	1	1
Department of Experimental Particle Physics (F-9)	162			3
Department of Inorganic Chemistry and Technology (K-1)	21		1	1
Department of Physical and Organic Chemistry (K-3)	32		1	3
Electronic Ceramics Department (K-5)	54		4	6
Department for Nanostructured Materials (K-7)	62		3	3
Department for Synthesis of Materials (K-8)	20		1	2
Department for Advanced Materials (K-9)	22			
Department of Biochemistry, Molecular and Structural Biology (B-1)	30			1
Department of Molecular and Biomedical sciences (B-2)	12	1		
Department of Biotechnology (B-3)	27		1	2
Department of Environmental Sciences (O-2)	118		1	2
Department of Automation, Biocybernetics and Robotics (E-1)	54			
Department of Systems and Control (E-2)	35	3	1	2
Artificial Intelligence Laboratory (E-3)	35	1		1
Laboratory for Open Systems and Networks (E-5)	25	2		1
Department of Communication Systems (E-6)	41			
Computer Systems Department (E-7)	19	1	1	
Department of Knowledge Technologies (E-8)	102			4
Department of Intelligent Systems (E-9)	70	2	1	2
Department of Reactor Engineering (R-4)	55	2		4
Reactor Infrastructure Centre (RIC)	8			
Networking Infrastructure Centre (NIC)		2		
Energy Efficiency Centre (EEC)	7			1
Centre for Electron Microscopy and Microanalysis (CEMM)	10			1
Centre for Knowledge Transfer in Information Technologies (CT-3)	3			
Milan Čopič Nuclear Training Centre (ICJT)	6			1
Radiation Protection Unit (SVPIS)	2			
Centre for Technology Transfer and Innovation (CTT)	2	1		
<b>Jožef Stefan Institute</b>	<b>1523</b>	<b>27</b>	<b>28</b>	<b>56</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.

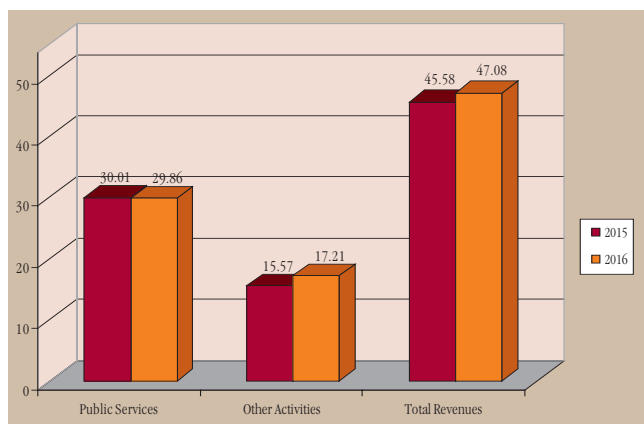
## R & D PROJECT PARTNERS

1. Adriaplin, Ltd., Ljubljana
2. Adriatic Slovenica, d. d., Ljubljana
3. Agency for Communication Networks and Services of the Republic of Slovenia, Ljubljana
4. Amebis, Ltd., Kamnik
5. Slovenian Agency for Radioactive Waste Management, Ljubljana
6. Bank of Intesa Sanpaolo d.d., Koper - Capodistria
7. Bioiks, Ltd. - Biomedical production with the finest quality, Ljubljana
8. C & G, Ltd. Ljubljana
9. Idrija Heritage Centre, Idrija
10. Chemass, Ltd., Ljubljana
11. The Centre of the Republic of Slovenia for Mobility and European Educational and Training Programmes (CMEPIUS), Ljubljana
12. Cosylab, d. d., Control System Laboratory, Ljubljana
13. Časnik Finance, Ltd., Ljubljana
14. Domel, Ltd., Železniki
15. DRI upravljanje investicij, Ltd., Ljubljana
16. Transparency International Slovenia, Ljubljana
17. Milan Vidmar Electric Power Research Institute, Ljubljana
18. ELES, Ltd., Electricity Transmission System Operator, Ljubljana
19. Elgoline, Ltd., Cerknica
20. ERICo, Ltd., Velenje
21. Flexatec, Ltd., Ljubljana
22. Fotona, Ltd., Ljubljana
23. GEN Energija, Ltd., Krško
24. Generali, d.d., Ljubljana
25. Goriška Local Energy Agency (GOLEA), Nova Gorica
26. Gorenje, d.d., Velenje
27. Hidria Rotomatika, Ltd., Spodnja Idrija
28. INEA, Ltd., Ljubljana
29. Informa Echo, Ltd., Ljubljana
30. Ecological engineering institute, Ltd., Maribor
31. Institute for Environmental Protection and Sensors (IOS), Ltd., Maribor
32. IPD Med, Ltd., Šentjernej
33. JP CCN Domžale-Kamnik, Ltd., Domžale
34. Kemomed, Ltd., Kranj
35. Agricultural Institute of Slovenia, Ljubljana
36. KMZ - Zalar Miran, s.p., Ljubljana
37. Knauf Insulation, Ltd., Škofja Loka
38. Kolektor Group, Ltd., Idrija
39. Komunala Novo mesto, Ltd., Novo mesto
40. LEK, d.d., Ljubljana
41. LPKF Laser & Electronics, Ltd., Naklo
42. L-TEK, Ltd., Šentjernej
43. Medens, Ltd., Mozirje
44. Merck, Ltd., Ljubljana
45. Metronik, Ltd., Ljubljana
46. Ministry of Finance of the Republic of Slovenia, Ljubljana
47. Ministry of Infrastructure of the Republic of Slovenia, Ljubljana
48. Ministry of the Interior of the Republic of Slovenia, Ljubljana
49. Ministry of Defence of the Republic of Slovenia, Ljubljana
50. Ministry of the Environment and Spatial Planning of the Republic of Slovenia, Ljubljana
51. Ministry of Justice of the Republic of Slovenia, Ljubljana
52. Ministry of Health of the Republic of Slovenia, Ljubljana
53. NELA razvojni center, Ltd., Železniki
54. Krško Nuclear Power Plant, Krško
55. Municipality of Zagorje ob Savi, Zagorje ob Savi
56. Optotek, Ltd., Ljubljana
57. Petrol, d.d., Ljubljana
58. Petrol, Ltd., Ravne na Koroškem
59. Plinovodi, Ltd., Ljubljana
60. Podkrižnik, Ltd., Ljubno ob Savinji
61. Quintelligence, Ltd., Ljubljana
62. Development Centre RC eNeM, Ltd., Zagorje ob Savi
63. Robotina, Ltd., Kozina
64. Sanolabor, d. d., Ljubljana
65. Saving, Ltd., Ljubljana
66. Scan, Ltd. Preddvor
67. Slovenian Biochemical Society, Ljubljana
68. Slovensko društvo ljubiteljev kemije, Ljubljana
69. Republic of Slovenia Statistical office, Ljubljana
70. Studio Moderna, Ltd., Zagorje ob Savi
71. Swatycomet, Ltd., Maribor
72. Špica International, Ltd., Ljubljana
73. TECOS, Celje
74. Unicredit Banka Slovenija, d.d., Ljubljana
75. University of Ljubljana, Ljubljana
76. University of Maribor, Maribor
77. University Rehabilitation Institute, Ljubljana
78. Ustna medicina, Ltd., Ljubljana
79. Vacutech Vakuumske tehnologije in sistemi, Ltd., Ljubljana
80. Xlab, Ltd., Ljubljana
81. Yaskawa Slovenija, Ltd., Ribnica
82. National Education Institute Slovenia, Ljubljana
83. ZEL-EN, Ltd., Krško
84. Zmas Group, Ltd., Ljubljana
85. Institute of Occupational Safety (ZVD), Ltd., Ljubljana

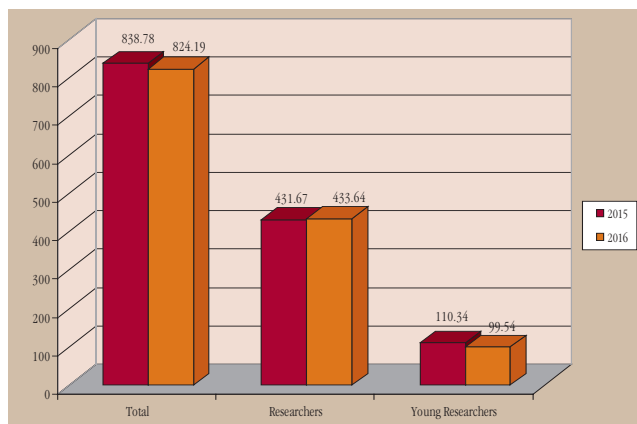
# INSTITUTE IN NUMBERS

2015-2016

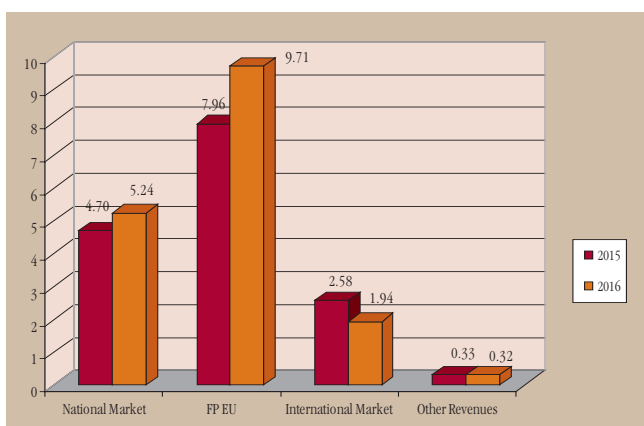
COMPARISON OF REVENUES (€M)



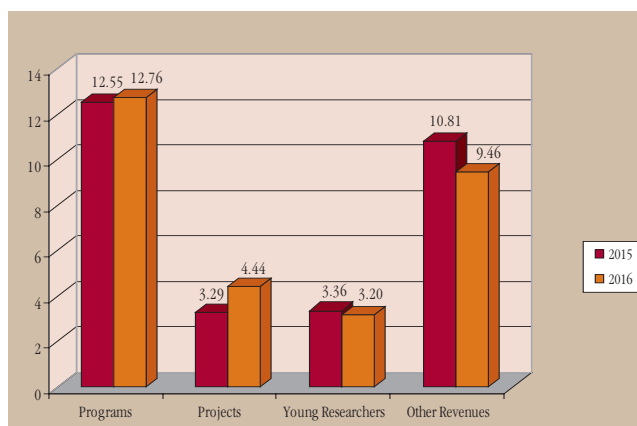
EMPLOYEES (FTE)



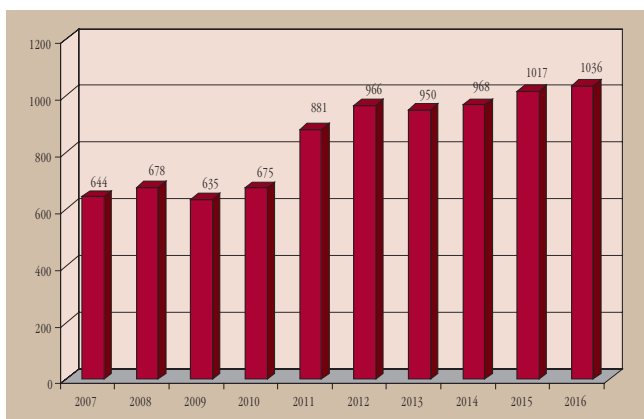
REVENUES FROM OTHER ACTIVITIES (€M)



REVENUES FROM PUBLIC SERVICES (€M)

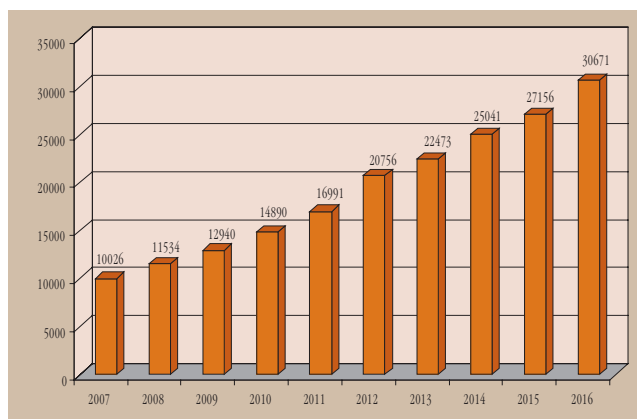


NUMBER OF PUBLICATIONS  
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\* retrieved 19 July 2017

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# RESEARCH DEPARTMENTS

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# DEPARTMENT OF THEORETICAL PHYSICS

F-1

*In 2016, members of the programme group THEORY OF NUCLEUS, ELEMENTARY PARTICLES AND FIELDS continued with their research in the area of hadronic physics, quantum chromodynamics, effective field theory of electroweak decays of mesons, unified theory and precise calculations in the three-body systems*

We have applied a coupled-channel formalism to calculate pion scattering and meson photo-production in eta N, K Lambda and K Sigma channels using a SU(3) version of the Cloudy Bag Model. With no additional free parameters pertinent to the strange hadrons, our amplitudes in the P11, P13, P33 and S11 partial waves agree well with the most recent partial-wave analyses. We have shown that our model is able to reproduce the free parameters of the Single Quark Transition Model.

A discovery of an intriguing exotic hadron, presumably composed of four quarks with different flavours X(5568), was reported by the D0 experiment in early 2016. We presented the first ab-initio theoretical study of the corresponding scattering channel  $B_s \bar{c}$  by means of the lattice QCD simulation. We did not find a candidate for this hadron, in agreement with the high-statistic LHCb experiment, which reported the results after we reached our conclusions.

We analysed the experimental hints of a diphoton resonance in the photon-invariant mass at 750 GeV in terms of a new boson, extracting information on its properties and exploring theoretical interpretations. We then showed how calculability and unitarity considerations severely limit the possible perturbative realizations of such a signal. Within the framework of the effective field theory, we also showed that in general two of the three processes  $S$  to  $ZZ$ ,  $S$  to  $Z$  gamma, and  $S$  to  $WW$  must occur with a non-zero rate. We also identified the most useful observables, whose relevance will also remain in model-by-model analyses. Finally, we explored the signal in the context of warped five-dimensional models with the Standard Model fields propagating in the bulk of the extra dimension as well as a bound system of a new QCD-like theory with massive fermions vectorial under the SM. We studied the phenomenology of light spin-0 particles and stressed that they can be efficiently searched for at the LHCb experiment in the form of dimuon resonances.

We have made an attempt to explain the LHC excess at 750 GeV using the scalar field that is a part of the SU(5) symmetry-breaking sector. Namely, in the adjoint representation of the SU(5) group, which breaks SU(5) down to  $SU(3) \times SU(2) \times U(1)$ , there is a Standard Model scalar. We also show that the required production and subsequent decay to two photons of this singlet can be induced by the individual or combined contribution of two scalar multiplets  $S_3$  and  $R_2$  that transform as  $(3, 3, -1/3)$  and  $(3, 2, 7/6)$  under  $SU(3) \times SU(2) \times U(1)$ , respectively.

According to the lattice QCD the mass spectrum of  $B_s$  mesons seems to follow the pattern of the  $D_s$  mass spectrum. As in the case of charmed mesons, the structure of positive parity  $B_s$  mesons is very intriguing. To shed more light on this issue, we investigated strong isospin violating decays  $B_s(0^+) \rightarrow B_s 0 \bar{c} 0$ ,  $B_s(1^+) \rightarrow B_s^* 0 \bar{c} 0$  and  $B_s(1^+) \rightarrow B_s 0 \bar{c} \bar{c}$  within the heavy meson chiral perturbation theory.

We showed that a model with a scalar leptoquark of hypercharge  $Y = 1/6$ , which includes the light right-handed neutrinos, can successfully describe both of the B-physics anomalies,  $R_{K\text{exp}} < R_{K\text{SM}}$  and  $R_{D\text{exp}} > R_{D\text{SM}}$ . We discussed the corresponding low-energy effective theory and, after using the known experimental data as constraints, we show that the model is viable and that it offers several predictions that can be tested experimentally.

We have shown that the violation of leptonic universality, as observed by the LHCb experiment in the decay  $B \rightarrow K \ell \ell$ , can be explained by the leptoquark with spin 1 and with a mass of around 1 TeV/c<sup>2</sup>. Furthermore, we also observed the lepton universality violation in charged-current



Head:  
**Prof. Sijetlana Fajfer**

**We analysed the experimental hints of a diphoton resonance in the photon-invariant mass at 750 GeV in terms of a new boson, extracting information on its properties and exploring theoretical interpretations.**

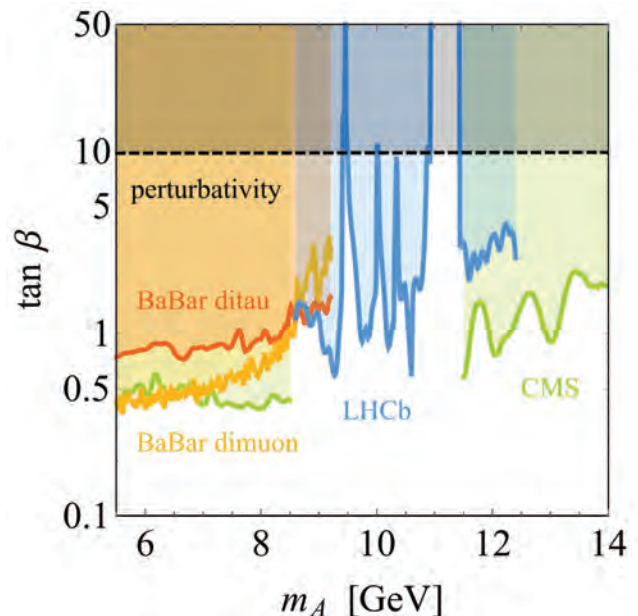


Figure 1: 95% CL bound on  $\tan\beta$  in the THDMII scenario. The blue curve follows from  $Y(n)$  production by LHCb, the green curve arises from a CMS dimuon resonance search, whereas the yellow and orange curves derive from the BaBar 90% CL limit on radiative  $Y(1)$  decays in the dimuon and ditau channel, respectively. The bound on  $\tan\beta$  arising from perturbativity is also shown (black dashed line). All the shaded regions correspond to excluded parameter space.

semitauonic decays  $B \rightarrow D^{(*)}\tau\nu$  compared to semileptonic decays with the light lepton  $B \rightarrow D^{(*)}l\nu$  can be explained with the presence of this leptoquark. The minimality of this model allows it to be predictable, and we have predicted the expected rate at which lepton flavour violating processes should be observed. The same leptoquark state has been analysed further in the systematic study of the connection between the lepton universality violation in  $B \rightarrow Kl$  and the lepton flavour violation.

In the invited review article “Physics of leptoquarks in precision experiments and at particle colliders” we have presented a broad overview of leptoquark physics. We discussed Standard Model extensions that contain leptoquarks and have focused on those leptoquark states that preserve the baryon number. For such states we have presented the most important constraints from precision measurements at low and high energies, the role of leptoquarks in Higgs physics as well as leptoquark searches at hadron colliders.

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**In an invited review article we presented a broad overview of the physics of leptoquarks, particles which switch between leptons and quarks.**

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We investigated a spontaneously broken  $U(1)_d$  gauge symmetry with a muon-specific dark Higgs. Our first goal is to verify how the presence of a new dark Higgs,  $\phi$ , and a dark gauge boson,  $V$ , can simultaneously face the anomalies from the muon magnetic moment and the proton charge radius. Secondly, by assuming that  $V$  must

decay to an electron-positron pair, we explored the corresponding parameter space determined by the low-energy constraints coming from Kaon, and tau physics. We focused on the scenario where the  $V$  mass is below  $\sim 2m_\mu$  and the  $\phi$  mass runs from a few MeV to 250 MeV, with  $V$ -photon mixing of the order  $\sim O(10^{-3})$ .

We restricted the soft terms of the minimal supersymmetric  $SU(5)$  to lie typically above 100 TeV with small  $\tan(\beta)$ . We found that the threshold corrections in the supersymmetric missing partner  $SU(5)$  suppress the  $D=6$  proton decay rate by 60%. We fit fermion masses and mixings with only one Yukawa matrix in a supersymmetric  $SO(10)$  with an extra vector-like representation 16. By comparing with data we found an agreement with the hypothesis of hidden residual symmetries in the Yukawa sector of  $SO(10)$  theories. We checked the possibility to have an ultraviolet fixed point in supersymmetric  $SO(10)$  and found some, not yet realistic, candidates.

The scalar sector of the minimal Left-Right model at the TeV scale is revisited. The stability and perturbativity of the effective potential is discussed and merged with constraints from low-energy processes. Lower limits on the triplet scalars are also derived: the left-handed triplet is bounded by oblique parameters, while the doubly-charged right-handed component is limited by the diphoton and photon-Z decays. Current constraints disfavor triples at the LHC as long as WR is within reach.

We have shown how to describe branes with an action that gives the geodesic equation in an infinite dimensional brane space with a certain metric. In analogy with general relativity we assumed that the metric can be a dynamical variable. Upon quantization of such a theory for the flat metric, we arrived at the quantum field theory of a continuous system of non-interacting scalar fields. The inclusion of a suitable interaction gives in the effective classical theory the equations of motion of a p-brane.

## Some outstanding publications in the past three years

1. Doršner, Ilja, Fajfer, Svjetlana, Greljo, Admir, Kamenik, Jernej, Košnik, Nejc. Physics of leptoquarks in precision experiments and at particle colliders. Physics reports, ISSN 0370-1573. [Print ed.], [in press] 2016, 68 str., doi: 10.1016/j.physrep.2016.06.001.

***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.***

Within the theory of correlated electrons we continued studies of many-body quantum states out of equilibrium. We addressed a long-standing problem concerning the origin of bosonic excitations that strongly interact with charge carriers, and show that the time-resolved pump-probe experiments are capable of distinguishing between phonons and magnons. The ability of phonon degrees of freedom to absorb unlimited amounts of energy renders relaxation dynamics nearly independent of the absorbed energy, while the hard-core effects pose limits on the spin subsystem resulting in a substantial dependence of the relaxation on the fluence. One of recent theoretical challenges is the phenomenon of the many-body localization, which predicts a nonergodic behaviour of disordered systems even in the presence of the interaction between particles. We have investigated several aspects of this problem within the disordered chain of interacting spinless fermions, revealing

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**It was shown that within a disordered Hubbard model, which simulates the experiments on cold-atom systems, spin degrees reveal an ergodic dynamics even in the presence of a strong disorder, while the charge degrees can localize.**

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an exponential vanishing of the d.c. conductivity with disorder, as well as universal dynamics in the vicinity of the transition. In the case of identical coupled chains we confirmed the breakdown of localization, consistent with recent experiments on disordered cold-atom systems. The latter were also the motivation for a study of the disordered Hubbard model, which showed that spin degrees of freedom behave ergodic even at strong disorder, while charges can localize, which is the indication of novel partial localization. We also studied the thermalization of an electron coupled to optical phonons and confirmed the approach to a thermal Gibbs ensemble.

Within the theory of quantum impurities and nanosystems we studied the sub-gap spectra of magnetic impurities in superconductors at finite temperatures. Experimentally, Shiba states have a finite width that emerges due to a normal-state tunnelling probe with a finite density of states, from experimental noise, but also from the electron-electron interaction, which was the focus of our research. We have explored the Kondo screening of localized moments in the extreme situation where the chemical potential is in the vicinity of a van Hove singularity and found that the resulting potential scattering strongly influences the renormalization of the exchange-coupling constant. We also derived an exact solution for a time-dependent wave function of an initial Kramers-doublet qubit, driven around a quantum ring. It was shown that the initial qubit may be transformed to an arbitrary point on the ring, which might result in an application in quantum computing.

We continued studies of the transport properties of materials with correlated electrons and studied the thermoelectric effect and the entropy in  $\text{Sr}_2\text{RuO}_4$ . In collaboration with an experimental group we investigated the THz optical conductivity of pseudocubic ruthenates. We implemented the calculation of optical conductivity in the LDA+DMFT. We investigated the transport properties in doped Mott insulators and explained them within the concept of bad metals. In collaboration with the laboratory for dielectric spectroscopy we also analysed the dielectric response of the ceramic system BZT.

Within the research of statistical physics of complex systems and networks, we have considered the nature of collective fluctuations using the multifractal time series analysis and algebraic topology of graphs, representing the transitions between states in the phase space. We have determined features of fluctuations that lead to an improved conductivity in nanostructured assemblies and the cooperative dynamics of the domain walls depinning. In the empirical data from the portal Mathematics, we have studied the growth of innovation in self-organized processes of knowledge creation through questions and answers. We also analysed multi-brain networks mapping the correlations among EEG signals, which are simultaneously recorded during the communications among the participants and have demonstrated that higher topological structures correlate with an understanding of the communicated contents.

## Some outstanding publications in the past three years

1. Mravlje, Jernej, Georges, Antoine. Thermopower and entropy: lessons from  $\text{Sr}_2\text{RuO}_4$ . Physical review letters, ISSN 0031-9007. [Print ed.], 2016, vol. 117, no. 3, str. 036401-1-036401-5, doi: 10.1103/PhysRevLett.117.036401.
2. Kogoj, Jan, Mierzejewski, Marcin, Bonča, Janez. Nature of bosonic excitations revealed by high-energy charge carriers. Physical review letters, ISSN 0031-9007. [Print ed.], 2016, vol. 117, iss. 22, str. 227002-1-227002-5, graf. prikazi, doi: 10.1103/PhysRevLett.117.227002.

***The group for THEORETICAL BIOPHYSICS AND SOFT-MATTER PHYSICS investigated polyelectrolytes, liquid crystals, colloids, and phospholipid and biological membranes.***

Our efforts in the field of macromolecular interactions and molecular biophysics included a range of problems and the most important ones are dedicated to the role of materials properties in van der Waals interactions, to the determination and analysis of the partitioning of differently sized polymers in membrane nanopores, and to the spectroscopic investigation of the role of magnesium ions on the details of the DNA structure in thin films. We also analysed the charge renormalization in asymmetric electrolytes, van der Waals interactions between layered media and

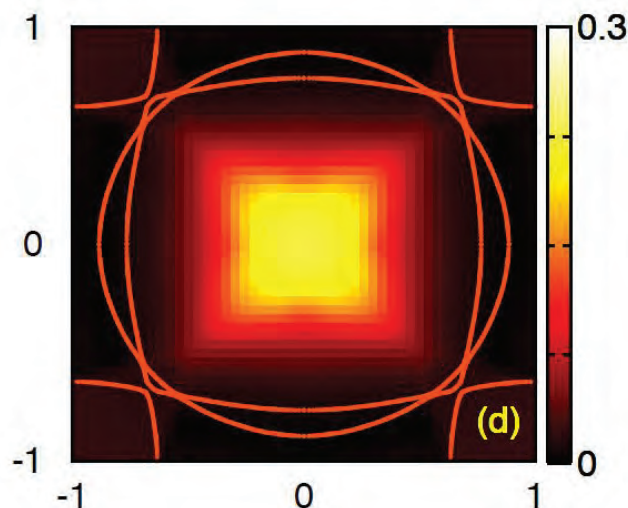


Figure 2: Fermi surface of a layered ruthenate  $\text{Sr}_2\text{RuO}_4$ . The colour encodes the magnitude of the current matrix element in the direction perpendicular to the layer, which leads to an explanation for the enhanced Seebeck coefficient in the  $c$ -direction.

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**We have delineated the most recent and comprehensive understanding of the van der Waals interactions in the context including soft matter and biophysics.**

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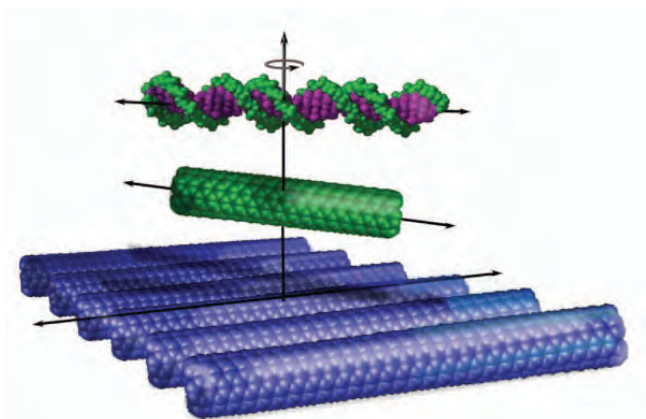


Figure 3: Van der Waals interactions are manifested in forces as well as torques between anisotropic molecules such as DNA and carbon nanotubes and molecular aggregates like the array of cylindrical molecules.

between polymers with sequence-specific polarizabilities, and fluctuation-induced forces in confined fluids and elastomers. In addition, we studied the stability of viral capsids, where we succeeded to relate the influence of long-range interactions with the elastic properties of viral capsids.

We studied the chiral structures and phases of bent-core liquid crystals, showing that the driving force for the formation of the modulated nematic phase are short-range steric interactions. We explained the optical activity of the nanofilament sponge phase, which stems from the layer inhomogeneity. We prepared a set of experiments for the analysis of optically positive and negative birefringent materials in the microwave region. Also developed was a systematic geometric interpretation of the symmetry of the crystals formed by model colloids with a step pair interaction.

We explored both experimentally and theoretically the self-replication of two-component lipid vesicles induced by heating, and we demonstrated that the observed self-replication mode depends on the asymmetric distribution of molecules in the two monolayers. A novel continuum formulation of the elastic behaviour of the red-blood-cell membrane skeleton was proposed and

used to analyse cell deformations that occur during its aspiration into a micropipette. We developed a mechanical theory of epithelial tissues, which was then used to interpret the shape of epithelial folds seen in the digestive tract and the airways of certain animals. Using the so-called thermomechanical analogy, we predicted the residual stress in the carotid artery.

## Some outstanding publications in the past three years

1. Woods, Lilia M., Dalvit, D. A. R., Tkatchenko, Alexandre, Rodriguez-Lopez, P., Rodriguez, A. W., Podgornik, Rudolf. Materials perspective on Casimir and van der Waals interactions. *Reviews of modern physics*, ISSN 0034-6861, 2016, vol. 88, iss. 4, str. 045003-1-045003-48, ilustr., doi: 10.1103/RevModPhys.88.045003.

## Awards and appointments

1. Prof. Dr. Jernej Fesl Kamenik: Zois recognition of achievements for the search for new physics in the theory of elementary particles, Ljubljana, Ministry of Education, Science and Sport.
2. Prof. Dr. Janez Bonča: Article in Nature Physics entitled: Snapshots of the retarded interaction of charge carriers with ultrafast fluctuations in cuprates, was selected as one of the most excellent scientific achievements in science in the year 2015.
3. Prof. Dr. Rudolf Podgornik: "Sackler Scholar", Israel, Mortimer and Raymond Sackler Institute of Advanced Studies, Tel Aviv University in the academic year 2016/2017, selected for "eminence in his field of research".

## Organization of conferences, congresses and meetings

1. Nonequilibrium Phenomena in Quantum Systems, Krvavec, 18.-21. 12. 2016

## INTERNATIONAL PROJECTS

1. COST CA15108; Connecting Insights in Fundamental Physics (FUNDAMENTALCONNECTIONS)  
Prof. Jernej Fesl Kamenik  
Cost Office
2. COST TD1210; Analysing the Dynamics of Information and Knowledge Landscapes  
Prof. Bosiljka Tadić  
Cost Office
3. H2020 - ITN - COLLDENSE; Hybrid Colloidal Systems with Designed Response  
Prof. Primož Ziherl  
European Commission
4. Search for Composite Higgs Models at the LHC  
Prof. Jernej Fesl Kamenik  
Slovenian Research Agency
5. Relaxation Dynamics and Thermalization of Quantum Many-body Systems  
Prof. Janez Bonča  
Slovenian Research Agency
6. Strong Electronic Correlations and Superconductivity  
Asst. Prof. Rok Žitko  
Slovenian Research Agency
7. From Flavor Anomalies to Signals in High-pT Searches  
Prof. Jernej Fesl Kamenik  
Slovenian Research Agency

8. Dark Side of the Higgs Boson  
Prof. Jernej Fesl Kamenik  
Slovenian Research Agency

## RESEARCH PROGRAMS

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

## R & D GRANTS AND CONTRACTS

1. Integrability and ergodic theory of non-equilibrium quantum many-body systems  
Dr. Jernej Mravlje
2. The many-impurity problem  
Asst. Prof. Rok Žitko
3. Thermodynamics of dissipative nanosystems  
Dr. Jure Kokalj

## VISITORS FROM ABROAD

1. Dr. Osor Slaven Barišić, Institut za fiziko, Zagreb, Croatia, 14.-15. 1. 2016
2. Prof. Masayuki Imai, Ochanomizu University, Tokyo, Japan 8. 2.-11. 2. 2016
3. Takuma Kono, Ochanomizu University, Tokyo, Japan, 8. 2.-11. 2. 2016
4. Ryuta Ebihara, Ochanomizu University, Tokyo, Japan, 8. 2.-11. 2. 2016
5. Fagner C. Correia, Institute of Theoretical Physics/UNESP Brazil, São Paulo, Brazil, 5. 2.-30. 7. 2016
6. Dr. Diego Correa, Universidad Nacional de La Plata, La Plata, Argentina, 12. 2. 2016
7. Dr. Sabyasachi Dasgupta, National University of Singapore, Singapore, 4. 3.-6. 4. 2016
8. Dr. Takumi Kuwahara, Nagoya University, Nagoya, Japan, 1.-31. 3. 2016
9. Dr. Robert Triebel, Technical University Graz, Graz, Austria, 29. 2.-3. 3. 2016
10. Dr. Aleksandr Azatov, ICTP, Trieste, Italy, 15. 3. 2016
11. Dr. Fady Bishara, Oxford University, Oxford, Great Britain, 22.-27. 3. 2016
12. Dr. Berislav Buča, Univerza v Splitu, Split, Croatia, 1. 4.-30. 6. 2016
13. Dr. Jacek Herbych, University of Heraklion, Heraklion, Greece, 4. 4.-12. 4. 2016 in 3.-14. 10. 2016
14. Prof. Dr. John H. Jefferson University of Lancaster, Great Britain, 19.-27. 4. 2016
15. Dr. Luiz Vale Silva, Universite Paris Sud, Orsay, France, 20.-22. 4. 2016
16. Prof. Dr. Sean Tulin, York University, Toronto, Canada, 9.-13. 5. 2016
17. Dr. Oleg Lebedev, University of Helsinki, Helsinki, Finland, 2.-6. 5. 2016
18. Dr. Willem-Victor van Gerven, Institut za fiziko, Belgrade, Serbia, 1.-30. 6. 2016
19. Jan Skolimowski, Institute of Theoretical Physics, University of Warsaw, Warsaw, Poland 16.-18. 5. 2016 in 3. 9. - 31. 10. 2016
20. Dr. Juan Carlos Vasquez Carmona, SISSA, Trieste, Italy, 16.-27. 5. 2016
21. Dr. Aielet Alfrati, Weizmann institute, Rehovot, Israel, 17.-20. 5. 2016
22. Dr. Olcyr Sumensari, Universite Paris Sud, Orsay, France, 23.-27. 5. 2016
23. Prof. Marcin Mierzejewski, University of Katowice, Katowice, Poland, 20.-29. 5. 2016
24. Dr. Ezequiel Alvarez, University of Buenos Aires, Buenos Aires, Argentina, 20.-26. 6. 2016
25. Dr. Darko Tanasković, Institut za fiziko, Belgrade, Serbia, 12.-18. 6. 2016
26. Prof. Dr. Leonid Glzman, University of Graz, Graz, Austria, 26.-27. 5. 2016
27. Dr. Pier Paolo Baruselli, TU Dresden, Germany in SISSA, Trieste, Italy, 31. 5. 2016
28. Dr. Adam Falkowski, Laboratory of Theoretical Physics Orsay, Universite Paris Sud, Paris France, 9.-14. 6. 2016
29. Dr. Mathias Pierre Laboratory of Theoretical Physics Orsay, Universite Paris Sud, Paris France, 9.-14. 6. 2016
30. Dr. Vid Iršič iz ICTP, Trieste, Italy, 23. 6. 2016
31. Dr. Matteo Lotito, University of Cincinnati, Cincinnati, USA, 27. 6. 2016
32. Dr. Josef Pradler, Austrian Academy of Sciences, Vienna, Austria, 7.-8. 7. 2016
33. Dr. Thomas Jacques, SISSA, Trieste, Italy, 14. 7. 2016
34. Miroslav Andjelković, Vinča Institute of Nuclear Science, Belgrade, Serbia, 14.-24. 7. 2016
35. Prof. Ross McKenzie, University of Queensland, Brisbane, Australia, 15.-26. 8. 2016
36. Dr. Admir Greljo, Universität Zürich, Physik-Institut, Zürich, Switzerland, 18.-26. 8. 2016
37. Dr. Banasri Basu, Indian Statistical Institute, Kolkata, India, 23. 8. do 26. 8. 2016
38. Sangeeta Rani Ujjwal, School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India, 11.-18. 9. 2016
39. Dr. Osor Slaven Barišić, Institut za fiziko, Zagreb, Croatia, 28. 9. 2016
40. Dr. Jure Zupan, CERN, Geneva, Switzerland, 18.-23. 10. 2016
41. Dr. Tanja Rindler-Daller, University of Vienna, Vienna, Austria, 13.-16. 10. 2016
42. Dr. Luca Tubiana, University of Vienna, Vienna, Austria, 30. 11. - 2. 12. 2016
43. Dr. Andrea Wolzter, CERN/EPFL, Geneva, Lausanne, Switzerland, 7.-8. 12. 2016
44. Dr. Marija Mitrović Dankulov, Institut za fiziko, Belgrade, Serbia, 27. 11. - 11. 12. 2016

## STAFF

### Researchers

1. Prof. Borut Bajc
2. Prof. Janez Bonča\*
3. Prof. Milan Brumen\*
4. Prof. Mojca Čepič\*
5. Prof. Svjetlana Fajfer\*, Head
6. Prof. Jernej Fesl Kamenik
7. Prof. Bojan Golli
8. Dr. Jure Kokalj\*
9. Dr. Nejc Košnik
10. Dr. Rajmund Krivec
11. Dr. Bing Sui Lu, left 16.08.16
12. Dr. Jernej Mravlje
13. Asst. Prof. Miha Nemevšek
14. Prof. Rudolf Podgornik\*
15. Asst. Prof. Anita Prapotnik Brdnik\*
16. Prof. Peter Prelovšek
17. Prof. Saša Prelovšek Komelj
18. Prof. Anton Ramšak\*
19. Dr. Tomaž Rejec\*
20. Prof. Bosiljka Tadić
21. Prof. Nataša Vaupotič\*
22. Prof. Primož Ziberl\*
23. Asst. Prof. Rok Žitko

### Postdoctoral associates

24. Dr. Nataša Adžić
25. Dr. Tilen Čadež
26. Dr. Jan Kogoj
27. Dr. Anže Lošdorfer Božič
28. Dr. Tjaša Švelc Kebe, left 01.02.16
29. Dr. Lev Vidmar

### Postgraduates

30. Andreas Kyriakos Doukas, B. Sc.
31. Darius Alexander Faroughy Carias, B. Sc.
32. Jakob Frontini, B. Sc.
33. Victor Francisco Guada Escalona, B. Sc.
34. Alen Horvat, B. Sc.
35. Matej Krajnc, B. Sc.
36. Dr. Žiga Osolin, left 01.07.16
37. Urša Škerbiš, B. Sc.
38. Lara Ulčakar, B. Sc.
39. Luiz Henrique Vale Silva, B. Sc.

### Technical and administrative staff

40. Nevenka Hauschild

Note:

\* part-time JSI member

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Nataša Adžić, Rudolf Podgornik, "Titratable macroions in multivalent electrolyte solutions: strong coupling dressed ion approach", *J. chem. phys.*, vol. 144, iss. 21, pp. 214901-1-214901-11, 2016.
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## REVIEW ARTICLE

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## SHORT ARTICLE

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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## UNIVERSITY, HIGHER EDUCATION OR HIGHER VOCATIONAL EDUCATION TEXTBOOK

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## MENTORING

1. Ana Gostinčar-Blagotinšek, *Inquiry-based teaching of physics-related topics in primary science*: doctoral dissertation, Ljubljana, 2016 (mentor Mojca Čepič).
2. Janez Urevc, *Characterizing the mechanical response of human carotid artery in physiological state*: doctoral dissertation, Ljubljana, 2016 (mentor Boris Štok; co-mentor Milan Brumen).
3. Nataša Adžič, *Varieties and phenomenology of electrostatic interactions in protein physics*: doctoral dissertation, Ljubljana, 2016 (mentor Rudolf Podgornik).

4. Urška Jelerčič, *Mechanical models of cell organelles*: doctoral dissertation, Ljubljana, 2016 (mentor Primož Zihel).
5. Jan Kogoj, *Microscopic mechanisms of ultra fast relaxation in correlated electron systems*: doctoral dissertation, Ljubljana, 2016 (mentor Janez Bonča).
6. Ambrož Kregar, *Spin-charge states in the presence of spin-orbit coupling*: doctoral dissertation, Ljubljana, 2016 (mentor Anton Ramšak).
7. Kristina Leskovar, *Ferroelectric smectic-A phase made of bent-core liquid crystals*: doctoral dissertation, Maribor, 2016 (mentor Nataša Vaupotič).
8. Žiga Osolin, *Strong correlations and magnetism in the Kondo lattice model*: doctoral dissertation, Ljubljana, 2016 (mentor Rok Žitko).
9. Maja Pečar, *Konoskopija in poučevanje anizotropnih optičnih lastnosti snovi*: doctoral dissertation, Ljubljana, 2016 (mentor Mojca Čepič).
10. Matej Erjavec, *Bottle model of colour vision*: master's thesis, Maribor, 2016 (mentor Nataša Vaupotič).
11. Neda Gačnik Čebulj, *Primary students' comprehension of density concept*: master's thesis, Ljubljana, 2016 (mentor Mojca Čepič).
12. Damjan Gašparič, *Measurements and Analysis of the Vertical Jump and its Use at the Physics Lessons in Primary School*: master's thesis, Maribor, 2016 (mentor Milan Brumen; co-mentor Robert Repnik).
13. Marko Rožič, *Video clip as a didactic accessory in physics classes*: master's thesis, Ljubljana, 2016 (mentor Bojan Golli).
14. Bernarda Urankar, *Active liquid crystal optical protective filter*: master's thesis, Maribor, 2016 (mentor Mojca Čepič).
15. Monika Hadalin, *Energy flow in a model of the solar collector*: master's thesis, Ljubljana, 2016 (mentor Bojan Golli).
16. Matija Kuclar, *Signali nove fizike v semileptonskih razpadih mezona B v stanja čarobnih mezonov s pozitivno parnostjo*: master's thesis, Ljubljana, 2016 (mentor Svjetlana Fajfer).
17. Črt Lozej, *Časovno odvisen transport naboja in toplote skozi kvantno piko*: master's thesis, Ljubljana, 2016 (mentor Tomaž Rejec).
18. Tadej Mežnaršič, *Laser Cooling of Cesium Atoms*: master's thesis, Ljubljana, 2016 (mentor Rok Žitko; co-mentor Peter Jeglič).
19. Jan Ornik, *Novel concepts for the detection of microplastics*: master's thesis, Maribor, 2016 (mentor Nataša Vaupotič; co-mentor Jan C. Balzer).
20. Klemen Pečnik, *Uporaba NMR spektroskopije in metod strojnega učenja za natančnejše iskanje biomarkerjev tumorskih celic*: master's thesis, Ljubljana, 2016 (mentor Primož Zihel; co-mentors Janez Plavec, Gregor Serša).
21. Lara Ulčakar, *Stabilnost magičnih razmerij prevodnosti majhnih grafenskih sistemov*: master's thesis, Ljubljana, 2016 (mentor Anton Ramšak; co-mentor Tomaž Rejec).
22. Marion Antonia van Midden, *Reconstruction of the intrinsic spectral function of the magnetic adatoms on superconductor surfaces from the differential conductance*: master's thesis, Ljubljana, 2016 (mentor Rok Žitko).

# DEPARTMENT OF LOW AND MEDIUM ENERGY PHYSICS

# F-2

*The Department of Low and Medium Energy Physics is engaged in research in the field of atomic and nuclear physics. The knowledge and expertise acquired in basic research is exploited for numerous applications, including radiological monitoring of the environment, in materials research, fusion, biology, energy storage, medicine, pharmacology, environment and archaeometry. Research is executed with our own instrumentation, consisting of ion accelerator and beamlines, dedicated detectors of ionizing radiation, experimental setups for atomic physics and calibrated radiation fields. In addition, researchers from the department are granted access to large scientific installations worldwide, including accelerators, synchrotrons, free-electron lasers, fusion reactors and plasma guns.*

In 2016, within the A1 Collaboration at the microtron MAMI (University of Mainz, Germany), we have continued with the measurement of quasi-elastic electron scattering on deuteron and carbon nuclei, in which we have used a polarimeter to detect the recoil proton polarization components. The purpose of both these measurements is to determine whether the nuclear environment (for example, by its increased local density) influences the elastic form factors of the nucleons and whether the polarization transfer to the outgoing proton is driven by some kinematic quantity, for example, the amount of the proton being off its relativistic mass shell.

We have continued our analysis of the method for the initial-state radiation (ISR) experiment and have submitted a paper for publication. The analysis of virtual Compton scattering at low momentum transfer, dedicated to the determination of generalized polarizabilities of the proton, and the analysis of electro-production of neutral pions in the energy region of the Roper resonance are also in their final stages. In addition, we completed the third production beam-time devoted to measurements of parity-violating electron scattering in which transversely polarized electrons are used and which offer a completely different sensitivity to the strange-quark content in the protons and their contribution to the electro-magnetic form-factors.

At the Thomas Jefferson National Accelerator Facility (Jefferson Lab) we have continued our measurement of real Compton scattering on the protons at high momentum transfers in the regime of the large Mandelstam variables  $s$ ,  $t$ , and  $u$ , as well as the second part of the experiment, which is aimed at determining the magnetic form-factor of the proton at high momentum transfers (up to  $18 \text{ GeV}^2$ ).

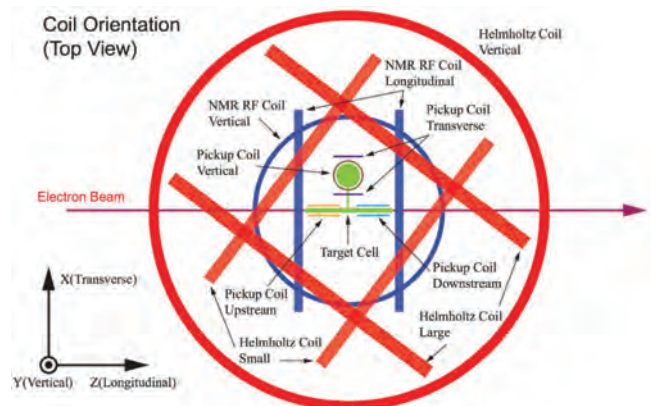
In 2016 we studied electron screening in the nuclear reaction between protons and deuterons at a proton beam energy of 260 keV. This reaction is important in the p-p chain, which dominates the energy production in the Sun and other similar stars. We were checking the hypothesis whether the resulting  $^3\text{He}$  emits an electron instead of a gamma ray. For this purpose we made an electron detection system for electron energies between one and ten MeV. Connected to our membership in the NUSTAR collaboration at the ESFRI infrastructure FAIR in Darmstadt, we proposed an experiment in which we would study isomeric excited states of heavy lead nuclei Pb-212, 214 and 216. In addition, we applied for a Slovenian-German bilateral cooperation project between JSI and centre FAIR. Within the proposed project, we would improve the active shielding of the DEGAS germanium detector array. Within the engagement at FAIR, we will host the NUSTAR collaboration annual meeting at JSI in 2017.

We have published several papers in the field of hadronic physics; the most important among them are the results of our study of eta and kaon production in chiral quark models (Golli in Širca, *Eur. Phys. Jour.* 2016), the report on measurements of  $d_2n$  and  $A_1n$  in order to probe the neutron spin structure (Flay et al. *Phys. Rev. D* 2016), the paper on the ground-state binding energy of  $^4\Lambda\text{H}$  hypernucleus from high-resolution decay-pion



Head:  
**Prof. Primož Pelicon**

**We continued the innovation work in the field of instrumentation in medical physics. A national patent "Angle-sensitive gamma camera with a rotary obstruction" was obtained in a close collaboration with the Institute of Oncology in Ljubljana. A connected patent is meanwhile undergoing a grant procedure in the United Kingdom.**



*Figure 1: The polarized  $^3\text{He}$  target setup used in several recent Jefferson Lab experiments dedicated to the study of neutron structure functions and investigations of electromagnetic and spin structure of  $^3\text{He}$ . The Helmholtz coils provide the holding magnetic field while the RF coils closer to the target cell are used for measurements of the degree of polarization by nuclear magnetic resonance techniques (Flay et al., *Phys. Rev. C*, 2016, 94, 052003).*

spectroscopy (Schulz et al., Nucl. Phys. A 2016), as well as on the electro-excitation of the  $\Delta(1232)$  resonance (Blomberg et al., Phys. Lett. B 2016).

We continued the innovation work at the field of instrumentation in medical physics. A national patent, "Angle-sensitive gamma camera with a rotary obstruction" Vencelj et al, SI 24818 A, WO 2016050631 A1, was granted for the work in a close collaboration with the Institute of Oncology in Ljubljana. Three system houses active in the market of medical instruments have so far inquired regarding the transfer of patent rights. A connected patent is meanwhile undergoing a grant procedure in the United Kingdom. A national patent "Process and a device for improvement of operation of silicon photomultipliers in the regime of piled-up pulses of light", Vencelj et al., SI 24863 A, WO 2016060622 A1, was granted for the result of a collaboration with Beyond Semiconductor LLC.

The Division of Ionizing Radiation Measurements was conducting the environmental radioactivity monitoring of the 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, monitoring of radioactivity in fodder, central radioactive waste repository radiological monitoring, monitoring of the radioactivity in drinking water, proficiency tests, material characterizations, calibrations of the radiation gauges and measurements of the personal and environmental doses by thermoluminescent dosimeters.

The Laboratory for Dosimetry Standards calibrated a number of measuring devices for radiation dose and ensured measurement traceability in the region. The listed laboratories active in the dosimetry of ionizing radiation are accredited according the standard SIST EN ISO/IEC 17025 and successfully performed at international intercomparisons in 2016. We participated in a number of international programmes and actions, including European Metrology Research Programme (EMRP), EURAMET, MODARIA II and CONCERT. We continued our activities on EMRP projects: "Metro materials with elevated natural radioactivity (MetroNORMprimo)" and "Metrology for radiological early-warning networks in Europe" (ENV57 MetroERM). Our main deliverable was the design and construction of a high-volume flow-rate air-pump with the embedded spectrometric system (Figure 1) for identification of the radionuclides in case of an incidental release. The system was tested in NPL, UK in spring 2016 and at intercomparison measurements at SCK-CEN in Belgium.

Members of the Infrastructure Group took part in regular drills and several special tasks with the radiological mobile unit ELME in Slovenia and participated at international comparison drills in Ronneburg, Germany, at intercomparison measurements at SCK-CEN in Belgium and at international regional drill of fire brigades in Venice.

In the field of theoretical atomic physics we focused our efforts on the development of the model for exact description of resonant decay in two-electron atoms within Exterior complex Scaling approach, as well as with the simulation of the effects of short intense light pulses through a dense gas. This was the foundation for the interpretation and the preparation for the experiments at Free Electron Lasers (FELs), where nonlinear effects need to be taken into account, such as many-photon excitations, and the inverse occupational states as a source of stimulated emission of hard ultraviolet (VUV) and x-ray light. Together with colleagues from the XFEL installation in Hamburg, we prepared an experiment proposal at FEL Flash in Hamburg, based on the open issues arisen at the last experimental campaign at FEL Fermi in Trieste. We want to understand, to what extent the observed stimulated emission in helium is a result of plasma processes, and if their role could be enhanced by excitation via short-lived double excited states. We took part at the experiment at FEL LCLS in Stanford, where we investigated short-lived transient states during the interaction of photo-excited complexes  $\text{Fe}(\text{CO})_5$  with ethanol solution. At the beamline SuperXAS of the SLS synchrotron in Villigen, Swiss, we executed similar experiment studying the interaction of

photo-excited molecules  $\text{CBr}_4$  with molecules of methanol solvent. In the time-stamped XANES we observed for the first time the intermediate product  $\text{HBr}$ , which indicates, that the present understanding of the reaction dynamics

**At the Free-Electron Laser (FEL) LCLS in Stanford we investigated short-lived transient states during the interaction of photoexcited complexes  $\text{Fe}(\text{CO})_5$  with an ethanol solution. We submitted an experiment proposal at FEL Flash in Hamburg, based on the open issues arising at the last experimental campaign at FEL Fermi in Trieste.**

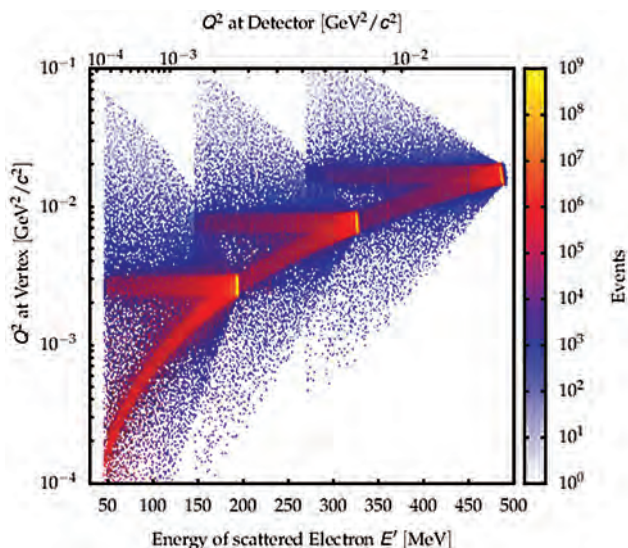


Figure 2: The figure presents the simulation for the Bethe-Heitler initial-state and final-state radiation processes which are being exploited to reach the information on the proton charge form-factors at extremely small four-momentum transfers. Shown is the distribution of events as a function of the momentum of the detected electron (horizontal axis) and the square of the four-momentum transferred from the virtual photon to the proton (vertical axis). In the initial-state radiation (ISR) process the incident electron emits a real photon before interacting with the proton; since the emitted photon carries away part of the incident energy, the momentum transferred to the proton is decreased. Hence, this process opens the possibility to probe the proton structure at extremely small values of  $Q^2$  that, using existing apparatus, could not be reached otherwise. (Mihovilović et al., AIP Conf.Proc. 2016, 1701, 040014).

**With methods RIXS, XANES and EXAFS, we were probing in operando the chemistry of Li-S and Mg-S batteries.**

should be redefined. At synchrotron Soleil we participated in the experiment with a magnetic bottle together with colleagues from the University Pierre and Marie Curie, where we studied Auger spectra from the photoionization of  $\text{SiH}_4$  and Na. In 2016, we published a study of exotic Auger transition of the Two-Electron-One Electron (TEOE) type, which was executed for the first time with high spectroscopic resolution for the case of double 2p vacancy in Argon (Žitnik *et al. Phys. Rev. A*, 2016). With approved beam time at the Galaxies beamline at Soleil, we will extend the research of TEOE to the molecular systems with Cl atoms. In the experiments executed at MaxLab in Lund in collaboration with partners from the University of Oulu, we showed that the decay of  $\text{CH}_3\text{Cl}$  leads to the fragments  $\text{HCl}^+$  (figure 3). We described the mechanism of molecular redistribution, which leads to the formation of these fragments (Kokkonen *et al. Phys. Rev. A*).

In the field of high-energy resolution x-ray spectroscopy two experimental runs have been performed at ID26 beamline of the ESRF synchrotron in Grenoble. In collaboration with the group from the Max Planck Institute for Chemical Physics of Solids from Dresden, we have performed resonant inelastic x-ray scattering (RIXS) measurements at the Ru- $L_{2,3}$  edges on  $\text{RuCl}_3$  ( $4d^5$ ) single crystal with a cubic local octahedral symmetry and at the Rh- $L_{2,3}$  edges on  $\text{Sr}_2\text{RhO}_4$  ( $4d^5$ ) single crystal with a distorted octahedral symmetry. RIXS spectroscopy provides  $L_{2,3}$  absorption spectra of 4d transition elements with energy resolution below the 2p core-hole lifetime broadening (HERFD technique), which is crucial to resolve the  $t_{2g}$  spectral component. In our experiment we have recorded Ru and Rh  $L_{2,3}$  HERFD spectra with energy resolution  $< 1\text{eV}$  and also their polarization dependence, which will provide a direct information about the purity of  $J_{\text{eff}}=1/2$  state of a low-spin (LS)  $4d^5$  configuration. In the second experiment performed in collaboration with the group from CEA in Grenoble, *in-operando* RIXS measurements at the sulphur 1s edge were performed on Li-S batteries to characterize the electronic structure of sulphur within the cathode material during the battery cycle. We were studying batteries where the  $\text{S}_8$  as the active material in the cathode is replaced by the  $\text{Li}_2\text{S}$ . The main problem in this case is high polarization in the first charge, which is not observed during the following ones. This might be due to differences in the particle size of raw  $\text{Li}_2\text{S}$  material (micron-sized) and the electrochemically produced one in a battery (nano-sized). In addition, we have performed also *ex-situ* RIXS and XAS measurements on magnesium-sulphur (Mg-S) batteries in collaboration with the group from the National Institute of Chemistry in Ljubljana. Among the potential sulphur-based batteries, the combination with Mg represents one of the most promising electrochemical couples. Mg-S batteries are still in the very early stage of research and development. Our experiment will contribute towards better understanding of complex electrochemistry within this novel type of high-energy-density batteries.

In 2016 we have published the results of *in-operando* RIXS measurements of sulphur within the Li-S battery, which were performed at ESRF in collaboration with the group from the National Institute of Chemistry in Ljubljana (Kavčič *et al., J. Phys. Chem. C* 2016). By using a selective resonant excitation the sensitivity for the lithium-polysulfide detection was significantly enhanced, while the sulphate signal from the electrolyte was heavily suppressed. This enabled a full quantitative analysis of separate sulphur compounds built up during the battery discharge (Figure 1). The results of our electronic structure study of phosphorus, sulphur, and chlorine in compounds with  $T_d$  and  $C_{3v}$  local symmetries performed by high-resolution K $\beta$  X-ray emission spectroscopy (XES) were published (M. Petric *et al., Inorg. Chem.* 2016). Measured spectra were reproduced by the model spectra of isolated  $\text{XO}_4^{n-}$  and  $\text{XO}_3^{n-}$  anions ( $X = \text{P}, \text{S}, \text{Cl}$ ) calculated within the density functional theory (DFT). The main spectral components were explained by the molecular orbital theory (Figure 2). We have also published the results of our theoretical and experimental studies of the structural and dynamical properties of chlorinated hydrocarbons performed by RIXS at the Cl 1s edge (Bohinc *et al., J. Chem. Phys.* 2016). The energy position, relative intensity, and the width of the Franck-Condon distribution of low-lying  $\sigma^*$  and  $\pi^*$  resonances were experimentally determined and compared with the theoretical values. In collaboration with the group from University of Helsinki we have published the results of our x-ray emission study of bulk aqueous sulfuric acid (J. Niskanen *et al., Sci. Rep.* 2016). We demonstrated

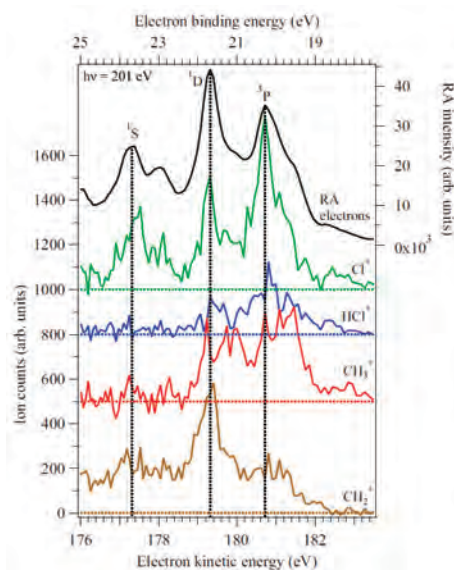


Figure 3: Distribution of the ionic fragments in coincidence with Auger electrons L-V2 after the photo-excitation of 2p electron in LUMO. The  $\text{HCl}^+$  fragment is formed from the specific final states V-2 only, with the energy of approx. 20 eV (Kokkonen *et al., Phys. Rev. A*, 2016, 94, 033409).

**Chemical shifts of the K $\alpha$  emission lines in X-ray spectra of P, S and Cl were systematically measured as a function of the chemical environment and reproduced within the numerical calculations using density functional theory.**

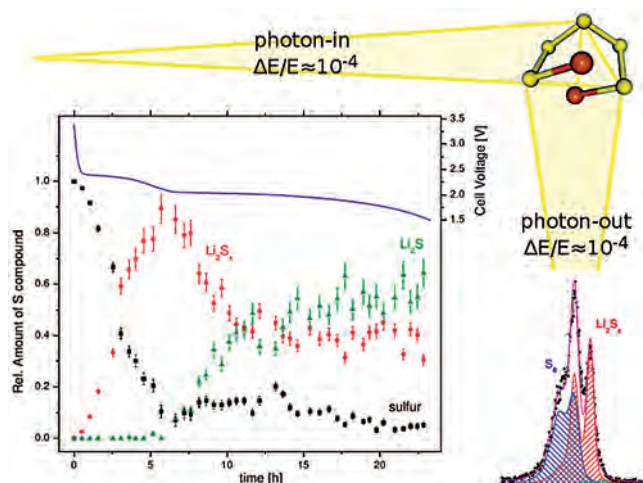


Figure 4: Relative intensity ratios of  $\text{S}_8$  and  $\text{Li}_2\text{S}_x$  compounds within the battery cathode during the discharge process together with the corresponding voltage diagram of the Li-S cell (M. Kavčič *et al., J. Phys. Chem. C* 2016, 120, 24568–24576).



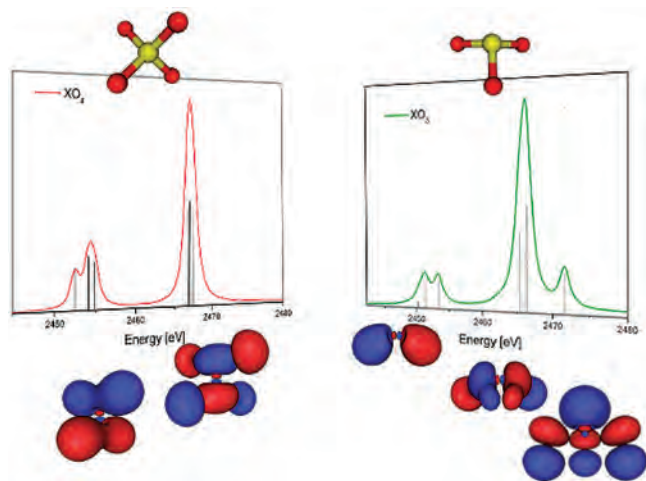


Figure 5: Theoretical  $K\beta$  x-ray emission model spectrum of the  $SO_4^{2-}$  in  $SO_3^{2-}$  ions with corresponding molecular orbitals building the main spectral components (M. Petric et al., *Inorg. Chem.* 2016, 55, 5328–5336).

that the S  $K\beta$  emission spectrum is a sensitive probe of the protonation state of the  $H_2SO_4$  molecule and can be used to determine quantitatively the fractions of different protonation states in the system.

In the field of proton-induced x-ray emission spectroscopy performed at the Microanalytical center, we have published the results of systematic experimental and theoretical study of chemical shifts of the characteristic K emission line of phosphorus, sulphur, and chlorine in different compounds covering the full range of oxidation states (Petric and Kavčič, *J. Anal. At. Spectrom.* 2016). The measured shifts reflect directly the effective local charge based on the DFT-calculated valence electron population and can be used to determine the oxidation state of the elements in various chemical environments, spreading the application of PIXE spectroscopy also towards chemical speciation. We have also published the results of the high-energy resolution  $K\beta_{1,3}$  x-ray emission measurements of Ar induced in collisions with 0.75–3.0 MeV protons (Kavčič and Banaš, *J. Phys. B: At. Mol. Opt. Phys.* 2016). Measured  $K\beta_{1,3}$ M satellite lines were used to extract the M shell single ionization probability for near-central collisions. Experimental values were compared with theoretical predictions. Good agreement was achieved with the values calculated within the semi-classical approximation using DHF wave functions for the description of valence M shell electrons.

The research with x-ray absorption spectroscopy was in 2016 performed at three synchrotron facilities: ELETTRA (Trst), PETRA III DESY (Hamburg) and ESRF (Grenoble). In collaboration with the National Institute of Chemistry, Ljubljana, a series of *in-operando* XANES and EXAFS experiments on high-energy-density Li-sulphur and Mg-sulphur batteries with various cathode materials and electrolytes 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 valence of sulphur, and the formation of Li- or Mg-polysulphides ( $Li_2S_x$ ,  $MgS_x$ ) compounds and finally crystalline  $Li_2S$  or  $MgS$  during discharge, and reversibility of the process during charging. This key information on the battery dynamics opened the way to an optimization of the synthesis of the material with maximum capacity.

In collaboration with Biotechnical Faculty of University of Ljubljana, Université catholique de Louvain (Belgium), Universitaet Bayreuth, Lehrstuhl Pflanzenphysiologie (Germany), ESRF Grenoble (France), National Agri-Food Biotechnology Institute (India), TU Berlin (Germany), we performed XAS experiments at PETRA III and at ESRF to determine the distribution of pollutant elements (Se, Hg, Cd, Pb) and essential elements (Zn, Cu, Ni, Mn, Fe) in cells to elucidate the molecular and cellular mechanisms which induce the tolerance to the noxious metal cations, or the mechanism of accumulation of essential elements in edible parts of the plants. With micro X-ray spectroscopy analysis at BLIX (TU Berlin) we investigated distribution of toxic elements on a cellular level. We published the results on Fe binding and distribution at the cellular and tissue levels in Tartary buckwheat, which revealed the effects of hydrothermal processing and germination on Fe speciation and Fe bio-accessibility to human intestinal cells (P. Pongrac et al., *Food chemistry* 2016). In addition we report on the strategy, how the roots of the metal-resistant plants cope with cadmium and zinc toxicities (I. Lefevre et al., *Plant and soil*, 2016), and on a study of Hg root uptake and ligand environment in fungi. In collaboration with University of Nova Gorica and National Institute of Chemistry, we continued long-term projects involving XANES and EXAFS measurements on the catalytic materials  $CeO_2$  doped with Cu and/or Zr, in operando during catalytic reaction at 400 C, and on  $TiO_2$  and  $SiO_2$  materials doped with Cu and/or Zr or Cr, Mn, Fe, Ni or Zn at room temperature. The valence of dopants and their atomic neighbourhood is determined to elucidate their catalytic properties. The materials aim to commercial applications

such as photo catalysis for water cleaning, adsorbents and ion traps, as well as a solid heterogeneous catalysts.

The collaborative work at the beamlines ALOISA and ANCHOR/HASPES (Laboratory IOM-CNR TASC) at synchrotron Elettra we investigated two-directional charge transfer at organic contacts. Using X-ray resonant photoemission spectroscopy we determined ultrafast charge transfer rates across pyridine/Au(111) interfaces, while also controlling the molecular orientation on the metal. We have shown that a bi-directional charge

transfer across the molecule/metal interface is enabled upon creation of a core-exciton with a rate that has a strong dependence on the molecular adsorption angle. These findings give an insight into the charge-transfer dynamics of photo-excited molecules at organometallic interfaces. (Cvetko et al., *Phys.Chem.Chem.Phys.* 2016).

In 2016, we continued with research in fusion, coordinated within EUROfusion Consortium within the Work Package on "Preparation of efficient Plasma-Facing Component (PFC) operation for ITER and DEMO". Major focus

**We experimentally demonstrated the synergistic effects of simultaneous structural defect creation and plasma bombardment in tungsten: hydrogen isotopes from plasma inhibit the defect annealing, and thus enhance the structural damage in the tokamak wall.**

of our research is the study of hydrogen-isotope retention in tungsten material, which is considered to be the most suitable material for plasma-facing components in future fusion reactors such as DEMO. The first important achievement was within the studies of the influence of material displacement damage on fuel retention, where high-energy ion irradiation is used as a surrogate for neutron damaging (Ogorodnikova et al., *J. Appl. Phys.* 2016). We made one step forward towards more realistic conditions by simultaneous defect creation by 10.8-MeV W-ion implantation and D-atom-beam exposure at five different temperatures between 450 K and 1000 K. Deuterium depth profile was measured by nuclear reaction analysis using  $D(^3\text{He},p)\alpha$ , which provides a measure of the defect density. The defects can retain hydrogen isotopes with high binding energy. Synergistic effects were observed as predicted by theory, i.e., higher D concentrations were found in the case of simultaneous damaging and D loading as compared to sequential damaging at elevated temperatures and D loading afterwards (figure 5) due to the stabilization of defects by the presence of solute hydrogen in the bulk.

Without the presence of hydrogen in the lattice the defects would namely annihilate at higher temperatures. (Markelj et al, *Nuclear Materials and Energy* 2017). The second achievement was on the subject to study the effect of He on hydrogen-isotope retention and transport, which was new in 2016. Recent experiments studying the interaction of hydrogen isotopes and helium with tungsten using He-seeded deuterium plasmas showed that He addition leads to reduced D retention. On the other hand, theory shows strong attraction between He and hydrogen, indicating preferential trapping of deuterium around implanted He clusters. In order to elucidate the possibility of He acting as a diffusion barrier or inducing preferential binding of hydrogen, we took an alternative experimental approach. He was implanted 1  $\mu\text{m}$  deep into a self-damaged tungsten to concentration of 4 at.%. Deuterium depth profiling was performed in-situ during isothermal annealing in the temperature range from 300 K to 800 K. It is shown for the first time that D accumulated in the He-implanted zone. D retention increased by a factor of two as compared to a non-He implanted tungsten reference. Rate equation modelling can explain the measured D depth profiles quantitatively when keeping the de-trapping parameters unchanged, but only increasing the number of traps in the He zone. This bolsters the confidence in the theoretical calculations predicting that more hydrogen can be stored around the He cluster zone. (Markelj et al, submitted to *Nucl. Fus. Lett.*). In 2016, an extensive study of the lateral distribution of D,  $^{11}\text{B}$  and  $^{15}\text{N}$  was performed by the use of focused ion beams on samples exposed in the divertor region of tokamak ASDEX Upgrade in nitrogen-15 seeding and He campaign.

With Mössbauer spectroscopy we studied  $\text{FePO}_4$  catalysts for the synthesis of methanol from methane with the addition of  $\text{O}_2$ ,  $\text{N}_2\text{O}$  in  $\text{H}_2\text{O}$  as oxidants. We determined the phase changes in fresh, reduced and spent catalysts. The Mössbauer data showed that the  $\text{Fe}_2\text{P}_2\text{O}_7$  phase is a dominating phase in the reduced catalyst. Cu-Fe oxide catalysts for partial CO oxidation (POX) in  $\text{H}_2$ -rich process streams have been studied. The Mössbauer data of the Cu and Fe loaded catalyst showed three well-defined sextets belonging to the tetrahedral and octahedral sites of  $\text{Fe}^{3+}$  ions.

At the JSI tandem accelerator, we enabled intense research work with high-energy ion beams in 2016. The accelerator delivered over 4000 beam hours to the users at the associated beamlines. In 2016, we initiated an upgrade of the beamline for the in-air beam applications. The insertion of the quadrupole lens and precise slits will allow us the formation of the in-air proton beam with diameter of 50 micrometres. This will enable us to measure the elemental maps with high lateral resolution at the field of archaeometry and biomedicine. With micro-PIXE method, we executed a series of measurements for the users from biomedicine. In collaboration with University Clinical Centre Maribor, we studied the clinical cases of failed hip prostheses. In selected cases, we observed high concentrations of wear metallic particles in the surrounding tissue sampled during the prosthesis replacements (Fokter et al, *Jour. Mech. Beh. Biom. Mat.* 2017). Within the collaborative work with University in Bayreuth (Detterbeck et al., *New Phytologist* 2016), we measured the distribution of nutrients and microelements in the grains of selected barley varieties (figure 7).

In the field of archaeometry, most attention was paid to the analysis of archaeological glass. We analysed a series of early medieval glass beads from the sites in Slovenia, which complement our measurements that were

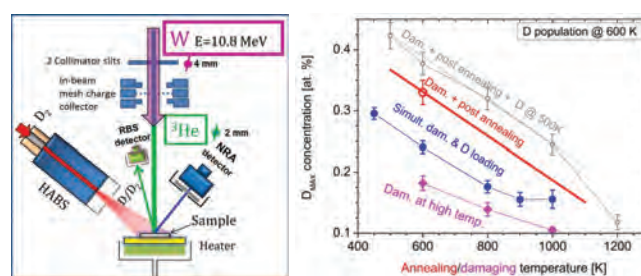


Figure 6: Left: Schematic figure of the INSIBA experimental set-up for simultaneous W-ion irradiation and exposure to atomic deuterium. Right: Maximum deuterium concentration versus annealing/damaging temperatures obtained from deuterium depth profiles on samples damaged at high temperatures and samples simultaneously damaged and deuterium loaded, respectively. The data are compared to results on samples damaged at room temperature and afterwards post-damaging annealed and defect populated by deuterium. (S. Markelj et al., *Nucl. Mat. Energy*, 2017).

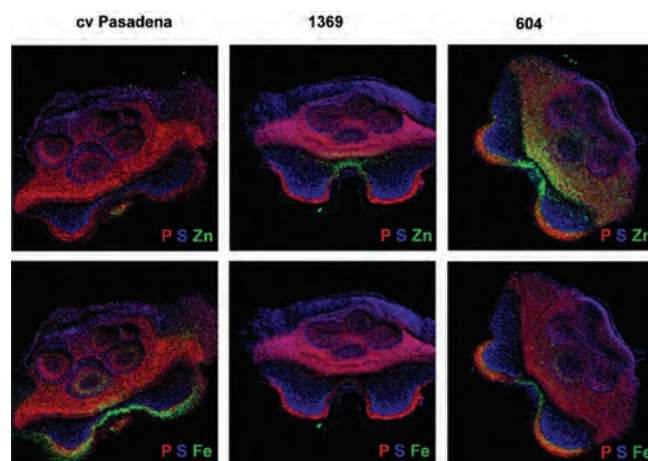


Figure 7: Co-localisation of zinc, iron, phosphorus and sulphur in the cross-section of barley seed, measured by micro-PIXE. From left to right: varieties "cv Pasadena", "1369" with low accumulation ability of zinc, and variety with high accumulation ability of zinc "604" (Detterbeck et al, *New Phytologist* 211 (2016), 1241).

already published in 2012. A detailed report for the magazine "Arheološki vestnik" is under preparation. Further, we measured a series of Late Antique glass from the site Gradina near Jelica in Serbia, which appears as a parallel to the site Tonovcov grad in Slovenia. However, important differences exist between the two sites, as the trace element pattern points to different sources of primary glass. We also contributed to the study of Venetian glass from Dalmatia and medieval Bosnia, which we do in collaboration with archaeologist Nikolina Topić from Dubrovnik and Rudjer Bošković Institute from Zagreb. As part of this work, we analysed a series of glass from medieval Bosnia and pointed out that the glass composition matches the original Venetian glass. Among the work, completed in previous years but published in 2016, we mention the study of pigments in the hand-painted autobiography of the Austrian diplomat Sigmund Herberstein printed in 1560. We found out that the pigments are based on the iron-gall ink, which has a harmful effect on the paper composition.

We continued the development of the MeV-SIMS method for molecular mapping of biology tissue. The existing method applying a pulsed primary ion beam was upgraded with an approach with a continuum primary beam. Within this upgrade, we install a channeltron that detects each individual arrival of primary ions. This configuration yields excellent lateral resolution of the molecular imaging, as well as better mass resolution due to a better time definition of the start signal. In collaboration with Maastricht University we studied the stigmatic imaging principle with the Time-Of-Flight (TOF) spectrometer for the MeV-SIMS case. For this purpose, we incorporate a TimePIX detector in the spectrometer, which combines both position sensitivity as well as fast timing characteristics required for TOF mass spectroscopy.

## Organization of conferences, congresses and meetings

1. MetroNORM Meeting, 23–24 February 2016, Ljubljana

## Patents granted

1. Matjaž Vencelj, Larisa Hosnar, Klemen Bučar, Janez Burger, Angle-sensitive gamma camera with a rotary obstruction, SI24818 (A), Slovenian Intellectual Property Office, 31. 03. 2016
2. Matjaž Vencelj, Miha Cankar, Andrej Likar, Process and device for improvement of operation of silicon photomultipliers in the regime of piled-up pulses of light, SI24863 (A), Slovenian Intellectual Property Office, 29. 04. 2016

## INTERNATIONAL PROJECTS

1. Calibrations  
Matjaž Mihelič, M. Sc.
2. TLD Dosimetria  
Boštjan Črnič
3. Extraction of Tantalum and Niobium from Ores  
Dr. Marijan Nečemer  
Prg Ltd.
4. FAIR Detectors  
Asst. Prof. Matej Lipoglavšek  
Gsi Helmholtzzentrum
5. 7FP - SPRITE, Supporting Postgraduate Research with Internships in Industry and Training Excellence  
Asst. Prof. Matjaž Kavčič  
European Commission
6. 7FP - PREPARE; Innovative Integrative Tools and Platforms to be Prepared for Radiological Emergencies and Post-accident Response in Europe  
Dr. Benjamin Zorko  
European Commission
7. MetroNORM; Metrology for Processing Materials with High Natural Radioactivity  
Branko Vodenik, M. Sc.  
Euramet E.v.
8. MetroERM; Metrology for Radiological Early Warning Networks in Europe  
Denis Glavič Cindro, M. Sc.  
Euramet E.v.
9. COST CM1204: XUV/X-ray Light and Fast Ions for Ultrafast Chemistry (XLIC)  
Prof. Matjaž Žitnik  
Cost Office
10. 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  
Asst. Prof. Sabina Markelj  
IAEA - International Atomic Energy Agency
11. RC 18353/R2; 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
12. RC 18186/R2; Application of Synchrotron Radiation in Studies of Environmental Impact on Biological Organisms; Experiments with Synchrotron Radiation for Modern Environmental and Industrial Applications  
Prof. Katarina Vogel-Mikuš  
IAEA - International Atomic Energy Agency
13. COST CA16117 - ChETEC; Chemical Elements as Tracers of the Evolution of the Cosmos  
Asst. Prof. Matej Lipoglavšek  
Cost Office
14. H2020 - CONCERT; European Joint Programme for the Integration of Radiation Protection Research  
Dr. Benjamin Zorko  
European Commission
15. Education-ED-FU, EUROFUSION  
Prof. Primož Pelicon  
European Commission
16. Plasma Facing Components-1-IPH-FU, EUROFUSION  
Asst. Prof. Sabina Markelj  
European Commission
17. Electromagnetic Structure of the Proton at High Momentum Transfers  
Prof. Simon Širca  
Slovenian Research Agency

## RESEARCH PROGRAMS

1. Archaeological and Archaeometric Research of Portable Archaeological Heritage  
Prof. Žiga Šmit
2. Structure of hadronic systems  
Prof. Simon Širca
3. Studies of atoms, molecules and structures by photons and particles  
Prof. Matjaž Žitnik
4. Object and Prestige; taste, status, power (Researches of the material culture in Slovenia)  
Dr. Marijan Nečemer

## R & D GRANTS AND CONTRACTS

1. Nanostructured cathodes for lithium sulphur batteries  
Dr. Darko Hanžel
2. Vegetation and hydrology of Ljubljansko barje in the past, present and future a consequence of succession, human impact or climatic fluctuations?  
Dr. Marijan Nečemer
3. 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
4. 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
5. Provision of Testing Services for Filter Media used in IMS Radionuclide Stations  
Dr. Benjamin Zorko  
The Preparatory Commission For The Comprehensive
6. Different Analyses  
Dr. Jasmina Kožar Logar

## NEW CONTRACTS

1. Ecology laboratory with mobile unit  
Asst. Prof. Matej Lipoglavšek  
Ministry of Defence
2. Annex No. 14 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
3. Maintenance of radiological emergency preparedness for a period of 5 years (2012-2017)  
Asst. Prof. Matej Lipoglavšek  
Krško Nuclear Power Plant
  4. Analyses of atmospheric releases in 2015, 2016 and 2017  
Dr. Benjamin Zorko  
Krško Nuclear Power Plant
  5. Environmental radioactivity monitoring of living environment in Slovenia in 2015  
Dr. Benjamin Zorko  
Ministry of the Environment and Spatial Planning
  6. Off-site radiological monitoring of the Krško Nuclear Power Plant in 2016 and 2017  
Dr. Benjamin Zorko  
Krško Nuclear Power Plant
  7. Environmental radioactivity monitoring of living environment in Republic Slovenia in 2016  
Dr. Benjamin Zorko  
Ministry of the Environment and Spatial Planning
  8. Measurement of gross alpha and beta activities in drinking waters in Republic of Slovenia  
Dr. Jasmina Kožar Logar  
Ministry of Health
  9. Monitoring of radioactivity in drinking water in Republic of Slovenia in 2016 and 2017  
Dr. Benjamin Zorko  
Ministry of Health
  10. Central radioactive waste repository radiological monitoring  
Dr. Marijan Nečemer  
ARAO - Agency for Radwaste Management, Ljubljana

## VISITORS FROM ABROAD

1. Dr. Thomas Schwarz-Selinger, Max Planck Institute (IPP), Garching, Germany, 20-25 March 2016
2. Prof. Dr. Chary Rangacharyuluja, University of Saskatchewan, Saskatoon, SK, Canada, 5. May 2016
3. Branko Petrinc, IMI, Zagreb, Croatia, 19. July 2016
4. Dr. Juegen Gerl, GSI, Darmstadt, Germany, 7-9 August 2016
5. Dr. Jelena Ajtić, The Faculty of Veterinary Medicine and Dr. Dragana Todorović, Vinča Institute, Belgrade, Serbia, 14-16 September 2016
6. Ivica Prlič and Branko Petrinc, IMI, Zagreb, Croatia, 7. December. 2016
7. Dr. Tim Vidmar in Jos Rutten, SCK-CEN, Mol, Belgium, 14.-16. 12. 2016
8. Dr. Luca Marchesi, Concettina Giovani in dr. Stefano Micheletti, ARPA FVG, Palmanova, Italy, 20. 12. 2016

## STAFF

### Researchers

1. Prof. Iztok Arčon\*
  2. Asst. Prof. Klemen Bučar
  3. Prof. Dean Cvetko\*
  4. Denis Glavič Cindro, M. Sc.
  5. Dr. Darko Hanžel
  6. Asst. Prof. Matjaž Kavčič
  7. Dr. Jasmina Kožar Logar
  8. *Dr. Peter Kump, retired 01.02.16*
  9. Asst. Prof. Matej Lipoglavšek
  10. Asst. Prof. Sabina Markelj
  11. Asst. Prof. Andrej Mihelič
  12. Dr. Marijan Nečemer
  13. **Prof. Primož Pelicon, Head**
  14. Prof. Simon Širca\*
  15. Prof. Žiga Šmit\*
  16. Asst. Prof. Matjaž Vencelj
  17. Branko Vodenik, M. Sc.
  18. Prof. Katarina Vogel-Mikuš\*
  19. Dr. Benjamin Zorko
  20. Prof. Matjaž Žitnik
- Postdoctoral associates**
21. Dr. Romana Krištof
  22. Dr. Miha Mihovilovič

23. Dr. Toni Petrovič
  24. Dr. Jelena Vesic
  25. Dr. Anže Založnik
- Postgraduates**
26. Žiga Barba, B. Sc.
  27. Tilen Brecej, B. Sc.
  28. Mateja Hrast, B. Sc.
  29. Boštjan Jenčič, B. Sc.
  30. Tim Kolar, B. Sc.
  31. *Nina Ogrinc Potočnik, B. Sc., on leave 01.06.14*
  32. *Marko Petric, left 01.09.16*
  33. *Samo Štajner, B. Sc., left 29.11.16*
- Technical officers**
34. Boštjan Črnič, B. Sc.
  35. Mitja Kelemen, B. Sc.
  36. Matjaž Mihelič, M. Sc.
  37. Primož Vavpetič, B. Sc.
- Technical and administrative staff**
39. Drago Brodnik
  40. Mojca Gantar
  41. Sandi Gobec
  42. Mirko Ribič, B. Sc.

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

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## REVIEW ARTICLE

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2. Benjamin Zorko, Matjaž Korun, Juan Carlos Mora Canadas, Valerie Nicoulaud-Gouin, Pavol Chyly, Anna Maria Blixt Buhr, Charlotte Lager, Karin Aquilonius, Pawel Krajewski, "Systematic influences of gamma-ray spectrometry data near the decision threshold for radioactivity measurements in the environment", *J. environ. radioact.*, vol. 158/159, pp. 119-128, 2016.

## SHORT ARTICLE

1. Denis Glavič-Cindro, Matjaž Korun, Branko Vodenik, Benjamin Zorko, "On the definition of the decision threshold as stated in the standard ISO 11929", *Accredit. qual. assur.*, vol. 21, no. 6, pp. 433-435, 2016.

## PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

1. Ivan Kreft, Blanka Vombergar, Paula Pongrac, Cheol Ho Park, Kiyokazu Ikeda, Sayoko Ikeda, Alena Vollmannová, Krzysztof Dziedzic, Gunilla Wieslander, Dan Norbäck, Vida Škrabanja, Igor Pravst, Aleksandra Golob, Lea Lukšič, Giovanni Bonafaccia, Nikhil K. Chrungeo, Meiliang Zhou, Katarina Vogel-Mikuš, Marjana Regvar, Alenka Gaberščik, Mateja Germ, "Coordinated buchwheat research: genetics, environment, structure and function", In: *The 13th international symposium on buckwheat (ISB): 2016. 9. 9. (Fri.) - 9. 11. (Sun.)*, [Korea], pp. 29-37.
2. Ivan Kreft, Blanka Vombergar, Paula Pongrac, Cheol Ho Park, Kiyokazu Ikeda, Sayoko Ikeda, Alena Vollmannová, Krzysztof Dziedzic, Gunilla Wieslander, Dan Norbäck, Vida Škrabanja, Igor Pravst, Aleksandra Golob, Lea Lukšič, Giovanni Bonafaccia, Nikhil K. Chrungeo, Meiliang Zhou, Katarina Vogel-Mikuš, Marjana Regvar, Primož Pelicon, Alenka Gaberščik, Mateja Germ, "Coordinated buchwheat research: genetics, environment, structure and function", In: *Strategies for improving the chronic diseases using buckwheat*, pp. 3-20.
3. Miha Mihovilovič, Harald Merkel, Adrian Weber, "Puzzling out the proton radius puzzle", In: *XIth Conference on Quark Confinement and Hadron Spectrum, 8-12 September 2014, Saint Petersburg, Russia*, (AIP conference proceedings, 1701), pp. 040014-1-040014-7.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Denis Glavič-Cindro, Drago Brodnik, Toni Petrovič, Matjaž Vencelj, Dušan Ponikvar, Steven J. Bell, Lynsey Keightley, Selina Woods, Stefan Neumaier, "MetroERM : Metrology for radiological early warning networks in Europe", V: *Proceedings, 25th International Conference Nuclear Energy for New Europe - NENE 2016, Portorož, Slovenia, September 5-8, 2016*, str. 1001-1-1001-10.
2. Bojan Golli, Simon Širca, "Puzzles in eta photoproduction: the 1685 MeV narrow peak: B. Golli and S. Širca", In: *Proceedings to the Mini-Workshop Quarks, Hadrons, Matter, Bled, Slovenia, July 3-10, 2016*, (Blejske delavnice iz fizike, vol. 17, no. 1), pp. 44-49.
3. Boštjan Jenčič, Luka Jeromel, Nina Ogrinc Potočnik, Katarina Vogel-Mikuš, Eva Kovačec, Marjana Regvar, Zdravko Siketič, Primož Vavpetič, Zdravko Rupnik, Klemen Bučar, Mitja Kelemen, Janez Kovač, Primož Pelicon, "Molecular imaging of cannabis leaf tissue with MeV-SIMS method", In: *The 22nd International Conference on Ion Beam Analysis (IBA 2015), June 14 - 19, 2015, Opatija, Croatia*, (Nuclear instruments & methods in physics research, Section B, vol. 371, 2016), pp. 205-210.
4. Matjaž Korun, Branko Vodenik, Benjamin Zorko, "Measurement function for the activities of multi-gamma-ray emitters in gamma-ray spectrometric measurements", In: *Proceedings of the 20th International Conference on Radionuclide Metrology and its Applications, 8-11 June 2015, Vienna, Austria*, (Applied radiation and isotopes, vol. 109, 2016), pp. 518-521.
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# DEPARTMENT OF THIN FILMS AND SURFACES

F-3

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

A few years ago we started to investigate two groups of nanostructured coatings: the nanolayer (AlTiN/TiN) and the nanocomposite (TiAlSiN). The work has always been performed in a parallel way: on the basic level we have been studying the coating growth mechanism and their properties, while on the applied level the emphasis has been on the applicability of these coatings for the protection of tools, used in a given production process. In the previous year, we primarily dedicated our work to the latter, i.e., the applied aspect. In collaboration with research partners from Turkey (University of Bartin), Serbia (University of Novi Sad) and Slovenia (Mechanical Engineering Faculty of the University of Ljubljana), and an industrial partner (EMO Orodjarna) we investigated the lifetime of these coatings for hard milling. We have been looking for an optimized structure substrate-coating in a stepwise fashion; last year a lot of work was dedicated to an improved cutting-edge geometry, specifically on a proper radius of curvature. This kind of research is typically conducted in a comparative way, where the standard TiAlN coating is taken as a reference (it has a homogeneous depth profile).

In addition to the cutting processes, we are also engaged in searching for the optimal protection of selected forming processes. In collaboration with the above-mentioned partners from Serbia, we are investigating the influence of CrN and CrAlN coatings for the protection of cores for the die casting of aluminium alloys. The wear mechanism of the tools protected in this way was the main topic of a PhD thesis by a candidate from that faculty; he performed most of the coating-related work in our lab. Aluminium die casting is a topic of several other informal collaborations with various Slovenian companies; there is work on die cores and knives for post-processing. We were also active on the technologically very challenging topic of the protection of tools for hot forging, where we tested the applicability of a CrVN coating. The idea is based on the superior tribological properties of vanadium oxide at high temperatures. For this purpose we analysed the oxidation mechanism for this coating and found that the principal diffusion paths for vanadium follow the growth defects.

The growth defects have been a topic of our department's research for several years. Last year the work was carried on in two principle directions. With partners from Croatia (Ruđer Bošković Institute) we compared the defect density and their internal structure in dependence on the type of deposition chamber used. In contrast to the previous experiments, which were performed in industrial chambers only, such kind of experiments was repeated in a laboratory chamber, which enables the deposition in a far cleaner environment. Nevertheless, the results showed that the density of small defects (size in the hundreds of nanometres) does not change substantially; this observation proves that the origin of the small defects is in the physical nature of the process, rather than in the secondary preparation.

The second direction of the last year concerns the question, what is the influence of growth defects on the initial stage of the tribological test? For this purpose we observed selected defects using a scanning electron microscope at different stages of the test. We found that the crushing of the growth defects – it appears after just a few laps of the contact surface – is the major source of abrasive particles. After the defects have been broken, the contact surfaces increase substantially and the system enters a stationary stage.

We concluded the project of testing the MoS<sub>2</sub> nanotubes as additives to classical lubricants. We performed several experiments on tribological systems protected by different hard coatings and evaluated the improvement of tribological properties. Last year we opened up a new direction of tribological research: conducting the experiments at high temperatures. With the installation of a new tribometer which enables measurements up to 1000 °C we will be able to track the coefficient of friction in realistic conditions, such as during hot forging, drilling, etc. As of today we have performed only a few preliminary experiments.

Magnetron sputtering is an established vacuum technique, which has been used for decades for the deposition of thin films. The process is based on plasma, acting as a source of ions to be accelerated towards



Head:  
**Asst. Prof. Miha Čekada**

**We showed that the addition of MoS<sub>2</sub> nanotubes to polyalphaolefin oil decreases the coefficient of friction in standard nitride coatings.**

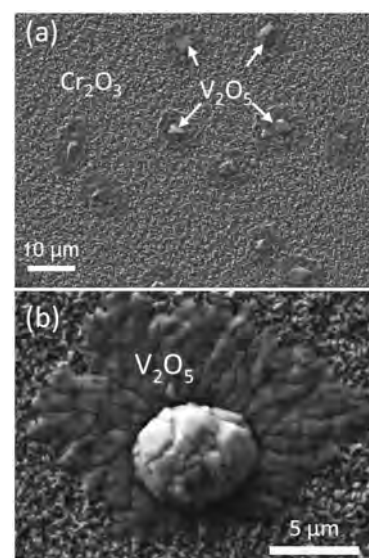


Figure 1: CrVN coating surface after oxidation. The vanadium diffusion takes place at the position of growth defects (a); detail of a single growth defect (b)



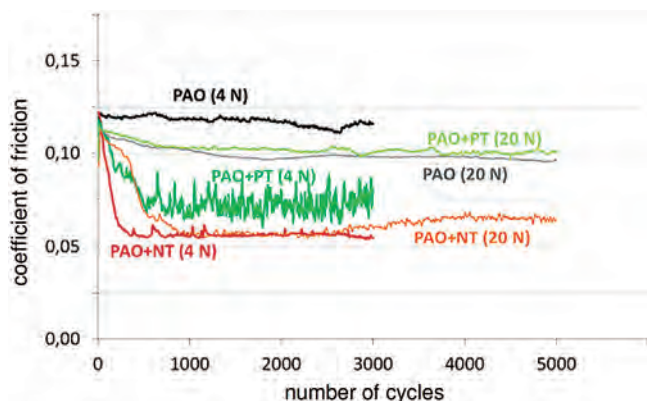


Figure 2: CrN coating coefficient of friction in polyalphaolefin oil (PAO), with MoS<sub>2</sub> powder addition (PT) and with MoS<sub>2</sub> nanotube addition (NT)

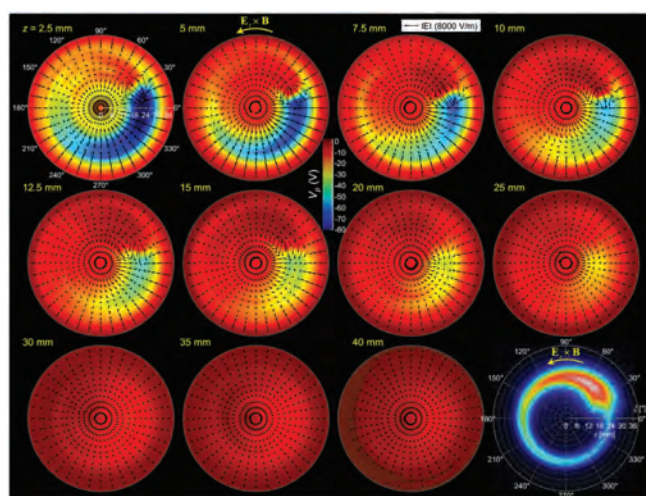


Figure 3: Plasma potential and electric field in magnetron plasma, measured at different axial distances from the cathode surface. The bottom-right image shows the ionization zone recorded by a high-speed camera. The position of the ionization zone approximately corresponds to the plasma potential distribution.

the target, and consequently to sputter the material around the vacuum chamber. The magnetron plasma appears homogeneous with a ring-like shape; however, the high-speed camera imaging showed that the plasma is concentrated in small areas, which were named the ionization zones. The zones have the shape of an elongated arrow, while their number depends on the discharge parameters. In previous years the department's coworker Dr. Matjaž Panjan investigated the properties of ionization zones in DC and pulsed magnetron sputtering. Among other results he showed that the plasma inhomogeneities have an important influence on particle transport in the plasma. In 2016 he measured the plasma potential of the rotating ionization zone using an emission probe. Using these measurements he was able to reconstruct the spatial distribution of the plasma potential, electric field, space charge and electron energy. These distributions enabled a deeper insight into the physics of elementary processes in magnetron sputtering. In collaboration with researchers from the Lawrence Berkeley National Laboratory (Berkeley, USA) he came to a conclusion that the electric field created by the ionization zone accelerates the charged particles and thus influences the ionization process and self-sustains the plasma. This conclusion differs from the commonly accepted hypothesis, that plasma is supported by secondary electrons only.

In addition to our core research topic - the study of hard protective coatings - we have always been at least partly active on some other fields of physics and chemistry of thin films and coatings. The following work should be mentioned:

- collaboration within the European project Eurofusion: deposition of WN thin films for studying ion-beam erosion, similar application with carbon layers, analytics of tungsten surface damages on the inner wall of a fusion reactor
- study of radiation damages during the laser ablation of surfaces, with a special emphasis on multilayer structures
- deposition of multilayer structures of Si/C for studying the diffusion processes
- study of magnetic properties of hematite nanoparticles in the amorphous silica matrix and calcium manganite nanoparticles
- analysis of surface topography for various applications: plasma-treated composites, electrochemically etched composites, optically variable refraction structures, printed oxide structures, etc.

This work was performed in collaboration with the following partners: Max Planck Institute of Plasma Physics, Garching, Germany; Vinča Institut for Nuclear Sciences, Belgrade, Serbia; Hungarian Academy of Sciences, Budapest, Hungary; National Institute of Chemistry, Ljubljana, Slovenia, and some others in a minor contribution.

Besides the above-mentioned research project we performed several analyses for different Slovenia companies: Cetus, EMO Orodjarna, IMP Pumps, Kolektor Sikom, Kovinos, Lama, LTH Castings, Phos in Tosama.

### Some outstanding publications in the past year

1. A. Drnovšek, P. Panjan, M. Panjan, M. Čekada, The influence of growth defects in sputter-deposited TiAlN hard coatings on their tribological behavior. *Surface & coatings technology*, 288 (2016), 171–178

## INTERNATIONAL PROJECTS

1. Microstructure, Morphology and Magnetism of Natural Hematite Crystallites and its Geological Significance  
Dr. Matjaž Panjan  
Slovenian Research Agency
2. Studies of Fundamental Processes in Magnetron Sputtering  
Dr. Matjaž Panjan  
Slovenian Research Agency
3. JET Campaigns-JET1-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. Understanding plasma processes and thin film growth in High Power Impulse Magnetron Sputtering  
Dr. Matjaž Panjan
2. Antibacterial Nanostructured Surfaces for Biological Applications  
Asst. Prof. Miha Čekada
3. Development and production of Taylor made milling tools, coatings and corresponding manufacturing technologies in individual tooling industry  
Asst. Prof. Miha Čekada
4. Self-lubricating and wear resistant PVD hard coatings based on (V,Cr,Al,Ti)N for hot-working processes  
Dr. Peter Panjan
5. Building blocks, tools and systems for the Factories of the Future – GOSTOP  
Asst. Prof. Miha Čekada

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3. Aleksandar Miletić, University of Novi Sad, Novi Sad, Serbia, 12.–21. 7. 2016
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6. Saša Kovačić, University of Zagreb, Zagreb, Croatia, 3.–7. 10. 2016
7. Vesna Damjanović, University of Belgrade, Belgrade, Serbia, 7.–10. 12. 2016
8. Marin Tadić, Vinča nuclear institute, Belgrade, Serbia, 7.–16. 12. 2016

## STAFF

### Researchers

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

### Postdoctoral associates

5. Dr. Srećko Paskvale, left 01.06.16

### Postgraduates

6. Aljaž Drnovšek, B. Sc.

7. Nastja Poljanšek, B. Sc.

### Technical officers

8. Uroš Stele, B. Sc.

### Technical and administrative staff

9. Joško Fišer
10. Damjan Matelič
11. Andrej Mohar
12. Tomaž Širnik

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# DEPARTMENT OF SURFACE ENGINEERING AND OPTOELECTRONICS

## F-4

**The research program is associated with vacuum science, technology and applications. The main activities are focused on plasma science, the modification of advanced biomedical materials and products for improved biocompatibility, the characterization of inorganic, polymer and composite materials with different thin films on the surface, the modification and characterization of 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 research team has built several plasma reactors in the past decade. The reactors are often made from glass in order to minimize the loss of neutral reactive gaseous species by heterogeneous surface recombination. Namely, the probability of such reactions on a smooth glass surface is low for most reactive particles. Gaseous plasma can be sustained by different discharges, but the team has specialized in electrodeless discharges powered by high-frequency generators. Small reactors are powered with microwaves, but for the sustenance of plasma in large reactors an electromagnetic field in the radiofrequency range performs better. Particularly suitable are both industrial frequencies of 13.56 and 27.12 MHz. A radiofrequency generator is coupled with a metallic coil wrapped on the glass tube. Such a configuration enables very good coupling between plasma electrons and the electromagnetic field in medium-size reactors, but stray effects are observed in large reactors where the plasma is sustained by powerful generators. In such cases stray effects are common and difficult to avoid. The unwanted effects are due to high voltages that appear across the coil at high powers. Such voltages cause stray capacitive coupling of the RF power to grounded metallic components as well as extensive radiation of the electromagnetic waves. Methods for suppressing high voltages, but keeping large powers, have been studied both theoretically and experimentally in the past few years and a patent application has been filed. The patent was granted in 2016 by the German Patent Office in Munich. In it we disclose methods for suppressing stray voltage across the plasma coil by the appropriate coupling of several coils. The invention relates to a device for the excitation of a high-frequency gas plasma, i.e., optimization of the transfer of electromagnetic power from a radio-frequency generator into a gas plasma. The transfer of power is optimized by using two or more parallel overlapping and offset excitation coils that are serially connected into the assembly, consisting of a generator, a high-frequency cable, a matching network and an excitation coil. The measurements on the connections of the excitation coil prove that for equal transfer of power a lower voltage is required on the double excitation coil consisting of overlapping excitation coils connected in parallel than on the ordinary excitation coil. With the same voltage on the connections of the coil, the plasma is also more intensive, if it is generated in two overlapping excitation coils connected in parallel.

The energy gained by charged gaseous particles oscillating in a high-frequency electric field depends on the mass of the particle. If a RF field is applied, the gaseous ions can hardly follow oscillations in the MHz range, so they gain negligible energy. Electrons are less massive and are accelerating in the field. If they gain enough energy they can multiply during ionization collisions with neutral molecules. The electric field in the coil has at least two components: the capacitive, which develops next to the powered part of the coil; and inductive, which develops inside the coil due to induced electric field. If the predominant component is capacitive, plasma is in the so-called "E-mode". The electric field in this mode is concentrated in a small volume so the density of electrons in gaseous plasma is rather low. In the opposite case the electric field occupies the entire volume inside the coil with a pronounced radial distribution and causes the acceleration of numerous plasma electrons. If the predominant coupling is inductive, the plasma is in "H-mode". The H-mode is characterized by a high electron density and bright luminosity. The appearance of the modes depends on several parameters, with the discharge



Head:  
**Prof. Miran Mozetič**

### The German patent office granted a patent on innovative coupling between an RF generator and gaseous plasma

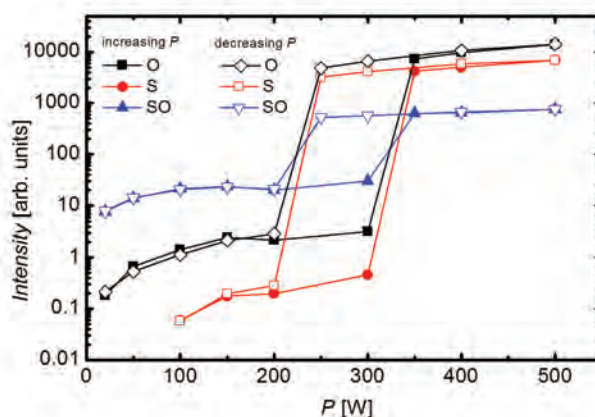


Figure 1: Hysteresis in OES intensities of S, O, and SO versus the forward RF power at a pressure of 30 Pa.

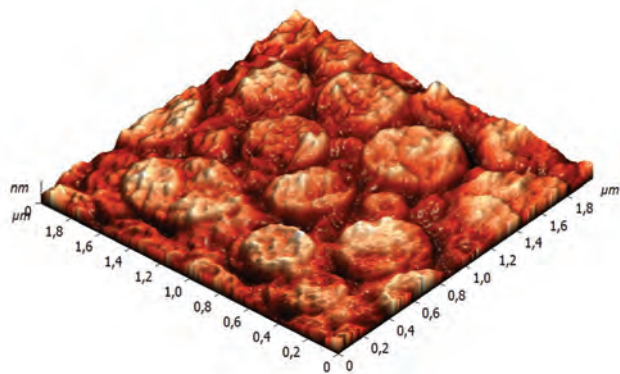


Figure 2: AFM image of originally smooth polymer surface after 80 s of treatment in  $H_2S$  plasma in the E-mode.

the enzyme inhibitor anti-thrombin; therefore, it is a beneficial coating on cardiovascular implants. A brief exposure of polyethylene terephthalate, a polymer commonly used for synthesis of artificial blood vessels, to  $SO_2$  plasma caused mild sulfurization, but atomic oxygen, which abounds in such plasma, causes continuous removal of sulfurized carbon, so the sulphur concentration on the polymer surface was hardly sufficient. Higher concentrations of sulphur on the surface of this polymer were found for the case that the plasma was created in  $H_2S$ . Depending on the plasma parameters the sulphur concentration as determined by X-ray photoelectron spectroscopy (XPS) reached almost 40 at.%. A well-pronounced maximum in the sulphur concentration versus the plasma treatment time was observed. A combination of XPS and time-of-flight secondary ion mass spectroscopy (ToF SIMS) techniques revealed the formation of polysulfide on the surface of PET polymer within a limited range of plasma radicals' fluence. The originally smooth polymer surface underwent an interesting change in the surface morphology. Within the limited range of the radicals' fluence, densely distributed circular nanostructures of typical sub-micrometre lateral dimension and a height of several 10 nm were observed by atomic force microscopy (AFM).

The plasma treatment causes changes in both surface morphology and functionality, which in turn influences the adsorption kinetic of proteins upon the incubation of polymeric grafts with human blood. This effect was studied in collaboration with a research team at Soleil synchrotron in France. Thin films of human serum albumin (HSA) were immobilized on polystyrene (PS) substrates previously functionalized either with polar or nonpolar functional groups. The functionalization was performed by treatment with cold gaseous plasma created in pure oxygen and tetrafluoromethane ( $CF_4$ ) plasmas, respectively. Samples were examined with soft

X-rays in the photon energy range of 520 to 710 eV in the ANTARES beam line. Near-edge X-ray absorption fine structure (NEXAFS) was selected for studying the behavior of albumin on the surface of a plasma-treated polymer. NEXAFS spectra of oxygen and fluorine K-edges were collected at different spots on the sample, and measurements at each spot were repeated many times. A strong degradation of the HSA protein upon irradiation with synchrotron light was observed. The weakly irradiated samples exhibited strong absorption at 531.5 eV associated with the  $O\ 1s \rightarrow \pi^*_{amide}$  transitions, and a broad non-distinctive peak at 540 eV was attributed to the  $O\ 1s \rightarrow \sigma^*_{C-O}$  transitions. Both peaks decreased with increasing irradiation time until they were completely replaced by a broad, non-distinctive peak at around 532 eV, indicating the destruction of the original protein conformation. The shortage of amide groups indicated breakage of the peptide bonds.

Low-pressure cold plasma is also useful for the treatment of textiles to improve their functional properties. A fruitful collaboration has been established with the Department of Textiles at the Faculty of Natural Sciences and Engineering, University of Ljubljana. Plasma created in various gases was used for both nanostructuring and functionalization of fabrics made from natural fibres. We were following the current trends of using ecologically benign treatments for surface finish as well as dyes extracted

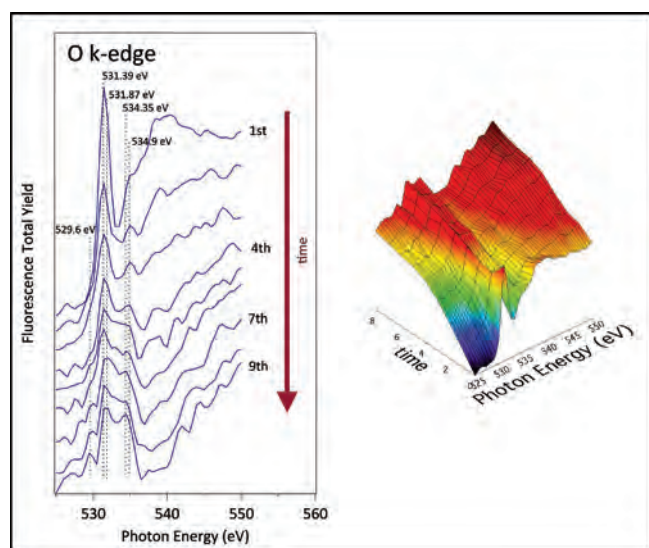


Figure 3: Series of oxygen K-edge NEXAFS spectra of an albumin-incubated sample treated with oxygen plasma and incubated with albumin.

from natural sources. In order to achieve colourful and antibacterial textiles, cotton and bamboo-rayon knitted fabrics were treated using radio-frequency, low-pressure plasma created in water vapour and dyed with the extract of *Fallopia japonica* (Japanese knotweed) rhizome. Water vapour was used as a natural choice since such fabrics contain a substantial amount of water, which is slowly released upon vacuum conditions. Even a brief plasma treatment induced a weak etching effect on the surface of the cellulose samples, since water molecules in plasma dissociate to produce hydroxyl radicals and oxygen atoms. Both radicals interact chemically with the organic material, thus interacting preferentially with any surface impurities as well as the uppermost layer of cellulose. Plasma-treated samples exhibited a higher dye uptake as well as pronounced antibacterial properties against *S. aureus*.

Another way to improve the performance of medical textiles is the incorporation of nanoparticles into fabrics or embedment into deposited coatings with antibacterial efficiency using atmospheric pressure plasma process. This research has been performed in the frame of the M-ERA.NET programme and strong collaboration with Ghent University. We developed a direct current plasma jet as a plasma-deposition source. The jet was stabilized by fast nitrogen flow. Three different types of the nanoparticles (silver, copper and zinc oxide) were employed as antimicrobial agents. During the deposition most of these nanoparticles were partially oxidized and embedded into the polymer coating generated by admixing hexamethyldisiloxane (HDMSO). The microbiological testing showed that samples loaded with nanoparticles of Ag and Cu and having a barrier layer of 10 nm, exhibit almost 97% bacterial reduction for *Escherichia coli* and *Staphylococcus aureus*, whereas the samples with ZnO nanoparticles provided only 86% reduction of *Staphylococcus aureus*.

Today, synthetic fibre-reinforced plastics have proven to meet the structural and durability requirements of components for various applications. However, glass-reinforced plastics exhibit shortcomings such as their relatively high fibre density, their difficulty to machine and poor recycling properties. With the growing global energy crisis and ecological risks, natural fibre-reinforced polymer composites have attracted more research interest due to their potential for serving as an alternative for artificial fibre composites. Natural fibres offer benefits such as reductions in weight, cost and CO<sub>2</sub> emission; less reliance on oil resources; and recyclability. To use the natural fibre-reinforced polymers, several major technical issues must be solved to facilitate the insertion of natural fibres in polymer composites. A critical factor in reinforced polymers is the strength of the bond between the fibre and polymer matrix, because the load is transmitted through the fibre-matrix interface. In order to improve it, we used the technology of selective plasma etching. An abundant natural source of fibres are coconuts. The raw coir fibres are not suitable for fibre-enforced plastics due to their hydrophobic nature since they contain lots of lignin and pectin. These components must be removed selectively from the fibres' surface to improve the adhesion of any polymer. Such an effect was achieved using rather aggressive oxygen plasma treatment. The impurities were quickly removed, revealing interesting structure of the coir fibres. Furthermore, the cellulose component was nanostructured so the treated fibres assumed excellent wettability – the water absorbency time decreased by two orders of magnitude.

Another good example of the selective etching of polymers and polymer-matrix composites is a collaborative work with the industrial partner Kolektor on an improvement of the insulating properties of polyphenolic composites. A composition with suitable fillers is a common strategy to improve the electrical insulation properties of polymeric materials, which is limited by the carbonization of a protruding surface polymer. To resolve this problem, we implemented Ar/O<sub>2</sub> plasma etching of a glass-filled polyphenolic composite to uncover the fillers by selective removal of the surface polymer. The exposure of the glass fillers increased the performance level to 65%, which enabled the material to be used as an insulator for commercial applications. The innovative solution to solving the problem of increasing surface insulation properties without adding expensive fillers to the polymer composite was also protected by a patent application.

Low-pressure, weakly ionized gaseous plasma is also suitable for tailoring the surface properties of inorganic materials. Within a newly granted project we studied the biological response of nanostructured titania that is suitable for the coating of vascular stents. Currently available stents are often made from titanium alloys. Such

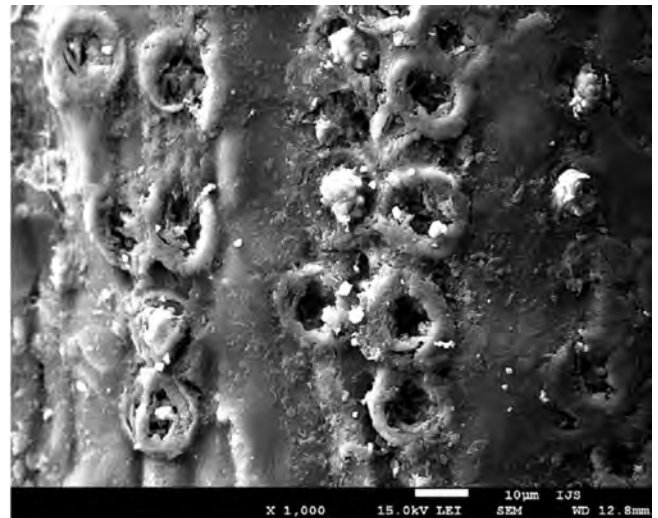


Figure 4: SEM image of a coir fibre after treatment with oxygen plasma reveals an interesting morphology.

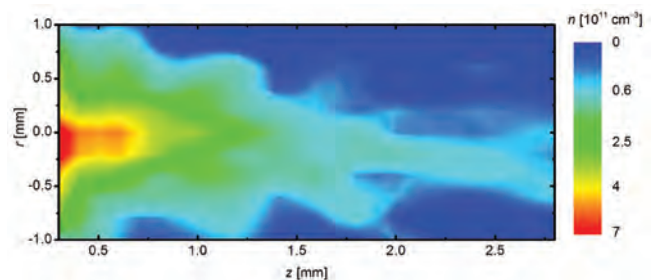


Figure 5: Spatially resolved He metastable density distribution over the effluent of a free atmospheric pressure plasma jet.

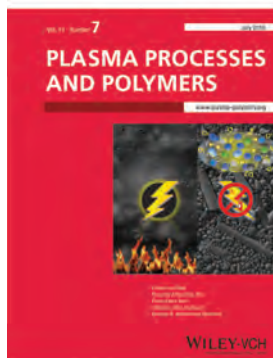


Figure 6: Journal cover page presenting improvement of plasma-etched thermoplastic composites, which become tracking and fire resistant.

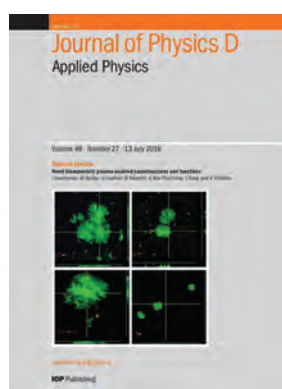


Figure 7: Journal over page presenting reduction of *P. aeruginosa* biofilm cells after plasma treatment.

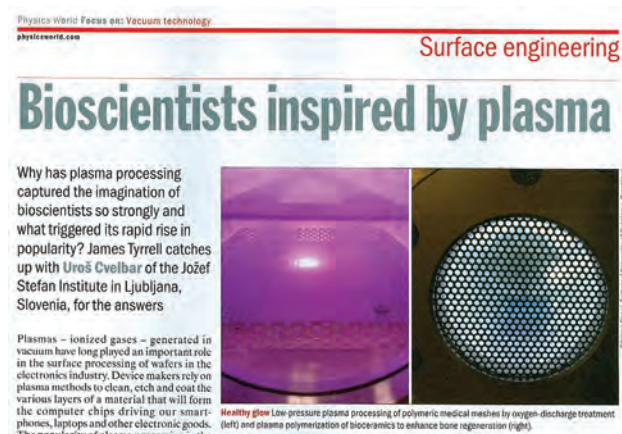


Figure 8: Promotion of special issue in *J. Phys. D: Appl. Phys.* on "Plasma-inspired biomaterials" edited by prof. Cvelbar.

stents lack of desired biological response, mostly due to restenosis, which occurs in more than 33% of cases where stents have been implanted. We developed a method for improving the proliferation of endothelial cells and simultaneously reducing adhesion and the activation of blood platelets on the surface of plasma-modified stents. The innovative method was disclosed in a patent application entitled: "Method for coating a medical device, especially a vascular stent" which has been submitted to the German patent office. We managed to achieve appropriate nanostructuring of the surface (biomimetic surface), which, after a treatment with highly reactive oxygen plasma, prevents platelet adhesion and activation, which in turn significantly reduces the possibilities for thrombotic reactions. Moreover, such a surface treatment also improves the endothelial cell proliferation, which is of primary importance, since such cells represent an ideal natural anti-thrombogenic material. In collaboration with the Faculty of Electrical Engineering, University of Ljubljana, we fabricated uniformly distributed dense and mechanically stable TiO<sub>2</sub> nanotubes on stents' surfaces. The plasma treatment enabled the removal of toxic fluorine, which is otherwise present on the surface due to electrochemical anodization process. *In-vitro* studies with whole human blood clearly showed that the platelets did not interact with surfaces prepared by the methods of invention, especially in the case of the 100-nm nanotube diameter. No platelets were detected on the plasma-treated TiO<sub>2</sub> nanotubes of 100 nm in diameter, and only a few on the nanotubes of 50 nm in diameter. Furthermore, *in-vitro* studies conducted with endothelial cells revealed the superior properties of plasma-treated nanostructured surfaces.

The stocks of fossil fuels are limited and their exploitation causes global warming, so we are looking for alternative energy sources for future generations. The cleanest energy arises from solar radiation, but it is difficult and expensive to transform it into useful energy. An alternative is the application of the same process as powers stars - nuclear fusion. Fusion power has the potential to provide sufficient energy to satisfy mounting demand, and to do so sustainably, with a relatively small impact on the environment. Nuclear fusion has many potential advantages over other energy sources. Firstly, its hydrogen isotope fuels are relatively abundant on earth. Furthermore, a fusion reactor would produce virtually no CO<sub>2</sub> or atmospheric pollutants, and its other radioactive waste products would be very short-lived compared to those produced by conventional nuclear reactors. Therefore, experimental fusion reactors have been built in order to solve numerous technological problems that currently prevent the exploitation of fusion energy. We have been involved in fusion-related research within Eurofusion projects for a decade. In 2016 we performed experiments at ASDEX Upgrade and JET reactors, which are currently the largest operating tokamaks. Our interest was mainly focused on ammonia production in fusion reactors. Because the cooling of the fusion plasma is needed near the plasma-facing components, nitrogen is often seeded into the divertor region. The ammonia is formed mainly in this region by surface processes. We investigated the production of ammonia on different materials currently used for manufacturing plasma-facing components in order to estimate the retention of tritiated ammonia in future reactors. This effect may be detrimental, but we discovered that ammonia also has at least one positive effect; it cleans amorphous hydrogenated carbon from the reactor walls.

The gas dynamics, in particular adsorption/desorption from walls of low-pressure reactors, is often studied by mass spectrometry. The precise quantification of extremely small gas amounts requires the applied quadrupole mass spectrometer to be *in-situ* calibrated at very small gas-leak rates. A precise calibration of a mass spectrometer was realized by leaking a specific gas through a fixed opening of the leak valve, connected to the analytical chamber. Exponential pressure decay in the upstream volume means that the molecular gas flow rate is also decaying exponentially. The correlation of the ion current of a specific ion mass versus the gas-leak

rate expresses the mass spectrometer's sensitivity over a wide range. During the calibration campaign conducted with hydrogen in an ultra-high vacuum (UHV) chamber, a slight deviation from the exponential decay and a drift of the base background pressure were observed. Both effects were attributed to the hydrogen absorption on surfaces. Its importance was then studied intentionally in detail. An UHV chamber is generally supposed to have a constant base background outgassing rate  $q_0$  over very long periods of time. In experiments with ionized or neutral molecular hydrogen, this level might be increased by the absorption of a small fraction of hydrogen. The absorption of molecular hydrogen was monitored in a small, austenitic stainless-steel UHV chamber during 3 h exposures at initial pressures from 0.01 to 1 mbar at room temperature. An absorbed dose of  $\sim 10^{13}$ – $10^{14}$  atom H cm<sup>-2</sup> was recorded. After gas removal, the desorption period in the closed vacuum system lasted for 20 h, wherein most of the absorbed hydrogen was released. The initial desorption rate was 10–100 times higher than the previous  $q_0$ . Calculations based on well-accepted

models for hydrogen-metal interactions confirm that the observed absorption-desorption processes are related mainly to the native oxide layer. Its reported thickness is between 1 and 3 nm, and our results express its high solubility, which at 1 nm ranges from  $K_{\text{sox}}(294\text{ K}) = 2.0 \times 10^{22}$  to  $3.8 \times 10^{22}$  atom H cm<sup>-3</sup>·bar<sup>-0.5</sup>. The recombination rate coefficient ranges from  $K_{\text{lox}}(294\text{ K}) = 8.9 \times 10^{-19}$  to  $6.45 \times 10^{-18}$  cm<sup>4</sup>s<sup>-1</sup>. The properties of the bulk metal were not affected noticeably in 24 h cycles as the oxide-layer-bulk-metal interactions proceed substantially slower.

Apart from low-pressure plasma we are also involved in research on non-equilibrium gaseous plasma created at atmospheric pressure. Although such plasma has several advantages over low-pressure plasma, the inadequate knowledge of its characteristics still prevents mass application on an industrial scale. An investigation of excited species, metastable states, reactive species, etc. is one of the highly desirable goals. Due to its important role in plasma generation and plasma chemistry processes, metastable helium (He) atoms are a great candidate for this kind of an investigation. We studied the properties of atmospheric pressure plasma jet (APPJ) in collaboration with our colleagues from the Institute of Physics in Zagreb, Croatia. Using cavity ring down spectroscopy (CRDS) we measured the density of He atoms in the metastable state ( $2^3S_1$ ), across the single electrode APPJ during the treatment of various samples. For the first time we managed to obtain the spatially resolved He metastable density distribution over the effluent of the APPJ. We found a correlation between sample conductivities and metastable He densities above the sample surface. The metastable He density can be increased with decreasing sample distance, increasing conductive sample surface area and by increasing He flow, which is important for the application of such plasma for tailoring the surface properties of materials on a small scale.

Atmospheric pressure gaseous plasma is not suitable for the uniform treatment of three-dimensional objects due to strong gradients in reactive particles densities, but performs well for the treatment of planar objects. The best results are obtained with porous two-dimensional products such as textiles. A technology for the treatment of infinite textiles used for wound healing has been developed in the frame of the EU project "IP4Plasma": Industrial Innovations Based on EU Intellectual Property Assets in the Field of Atmospheric Pressure Plasma Technology. The project was completed successfully in the autumn of 2016. The IP4Plasma project was funded by the European Union under the 7<sup>th</sup> Framework Programme for Research and Innovation. It lasted three years and involved some leading experts in surface engineering by gaseous plasma, equipment manufacturers and users of plasma technologies. Nine European partners from research organizations and industry were involved: Spinverse Ltd (Finland), Fraunhofer Institute for Surface Engineering and Thin Films IST (Germany), IMA (Belgium), Jozef Stefan Institute (Slovenia), LIONEX GmbH (Germany), SOFTAL Corona & Plasma GmbH (Germany), Tosama (Slovenia), VITO - Flemish Institute for Technological Research (Belgium) and 2B (Italy). The result of this project is a new technology for the plasma deposition of coatings on wound dressings, improving the wound-draining behaviour and add anti-inflammatory properties of products made by Tosama company. Our group performed a precise surface characterization of plasma-deposited coatings using the XPS and ToF-SIMS methods. In the frame of the project we also developed a new method for the fast and in-line monitoring of the efficiency of the air plasma surface activation at very high speed of textiles, which has a great potential for global industrial applications.

Similarly, the control and regulated release of antibiotic drugs from plasma-treated medical implant surfaces could be achieved using atmospheric plasma sources. Calcium phosphate ceramics are promising bone substitutes, since they have good biocompatibility and bioresorbability. Currently, such ceramics loaded with antibiotics in order to prevent infections are already on the market, but the control of release patterns has to be further improved. Cold plasmas can provide useful means of modifying the surface interactions with drugs through surface modification. For this reason, we explored the possibilities of using atmospheric pressure plasmas as a tool for modifications of calcium phosphate materials with newly



Figure 9: An atmospheric pressure plasma reactor was integrated to the production line at Tosama company for the deposition of antimicrobial thin films on wound care products in the frame of the European project IP4Plasma

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**The European project IP4Plasma involving nine European partners, among them the Jožef Stefan Institute and the Tosama company from Slovenia, was completed successfully**

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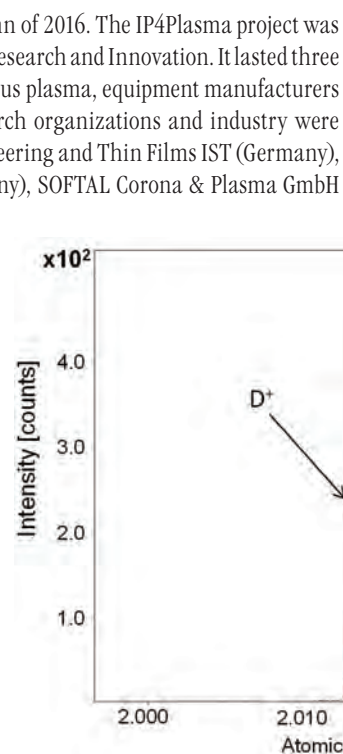


Figure 10: High-resolution mass spectra obtained by the ToF-SIMS method from diamond-like carbon after the desorption of a lubricant containing deuterated hexadecanol molecules.



populated bonds and charges, with the aim of enabling higher loading and controlled drug release. For surface modifications of  $\beta$ -tricalcium phosphate ceramics we implemented APPJ sustained in helium as a tool for tuning the controlled release of the antibiotic doxycycline hyclate, employed as a drug model. The surface chemistry was tailored upon interaction with the APPJ. We managed to obtain an increased oxygen-to-carbon ratio without changes in the topography as well as a build-up of surface charges. This led to slower and steady release kinetics after bonding drugs to the surface. Moreover, we demonstrated that atmospheric pressure plasma might prove to be a promising new tool that will lead to the design of a better controlled drug release from bio-ceramic matrices.

Diamond-like carbon (DLC) films are one of the fastest developing coatings ensuring low friction and protecting the sliding surfaces of various mechanical components. Because of their superior sliding properties, DLC coatings are now being widely used in many applications such as IC engines, slider bearings and hard discs. Despite the good sliding properties, even in the absence of any lubricant, the use of a lubricant seems inevitable for better heat dissipation and thus extended service life. The interaction between lubricants and DLC coatings is still not well understood, despite many studies over the past few years. We used ToF-SIMS and XPS methods to examine the adsorption ability and mechanisms with respect to two oiliness additives, i.e., hexadecanol and hexadecanoic acid, on the surface of weakly oxidized DLC coatings. Additionally, we analysed the resistance of the adsorbed additive films against external influences. Neither of these surface-sensitive techniques is capable of distinguishing between hydrogen from the substrate and the additives. In order to obtain impeccable results, the additives were deuterated. The high resolution of the ToF SIMS instrument allowed for a distinction between deuterium atoms from the additive and hydrogen molecules from the substrate in secondary-ion spectra. Our results show that both



Figure 11: The JVC-16 & EVC-14 conference attracted 181 participants from 25 countries.

molecules adsorb on the surface oxides and hydroxides and shield these structures with their hydrocarbon tails. This makes the surfaces less polar, which was manifested in a smaller polar component of the surface energy. Of the two examined molecules, the hexadecanoic acid showed a greater adsorption ability than the alcohol, which explains the better tribological properties when the acid was used as an additive in a lubrication oil.

The research team organized several international scientific meetings including the 16<sup>th</sup> Joint Vacuum Conference (JVC-16) and the 14<sup>th</sup> European Vacuum Conference (EVC-14). The conference took place in Portorož between June 6<sup>th</sup> and 10<sup>th</sup>.

### Some outstanding publications in the past three years

1. Vesel, A.; Mozetic, M.; Zaplotnik, R., Device for high-frequency gas plasma excitation: DE 112012000015 (B4), 2016-04-21. *Munchen: Deutsches Patent Office* 2016.
2. Zaplotnik, R.; Vesel, A.; Mozetič, M., Investigation of reactive plasma species created in  $\text{SO}_2$  by an inductively coupled RF discharge in E- and H-mode. *Journal of applied physics*, 2016, 120, 163302-1-163302-9.
3. Recek, N.; Primc, G.; Vesel, A.; Mozetič, M.; Avila, J.; Razado-Colambo, I.; Asensio, M. C., Degradation of albumin on plasma-treated polystyrene by soft X-ray exposure. *Polymers*, 2016, 8, 244-1-244-7.
4. Gorjanc, M.; Savič, A.; Topalič-Trivunović, L.; Mozetič, M.; Zaplotnik, R.; Vesel, A.; Grujić, D., Dyeing of plasma treated cotton and bamboo rayon with Fallopija japonica extract. *Cellulose* 2016, 23, 2221-2228.
5. Drenik, A.; Mourkas, A.; Zaplotnik, R.; Primc, G.; Mozetič, M.; Panjan, P.; Alegre, D.; Tabarés, F.L., Erosion of a-C:H in the afterglow of ammonia plasma. *Journal of Nuclear Materials* 2016, 475, 237-242.
6. Zaplotnik, R.; Biščan, M.; Popović, D.; Mozetič, M.; Milošević, S., Metastable helium atom density in a single electrode atmospheric plasma jet during sample treatment. *Plasma Sources Science and Technology* 2016, 25, 035023.
7. Simič, R.; Kalin, M.; Kovač, J.; Jakša, G., Adsorption of alcohols and fatty acids onto hydrogenated (a-C:H) DLC coatings. *Applied Surface Science* 2016, 363, 466-476.
8. Canal, C.; Modic, M.; Cvelbar, U.; Ginebra, M.P., Regulating th antibiotic drug release from  $\beta$ -tricalcium phosphate ceramics by atmospheric pressure surface engineering. *Biomaterials science* 2016, 5, 1454-1461.
9. Puliyalil, H.; Slobodian, P.; Sedlacik, M.; Benlikaya, R.; Riha, P.; Ostrikov, K.; Cvelbar, U., Plasma-enabled sensing of urea and related amides on polyaniline. *Frontiers of Chemical Science and Engineering* 2016, 10, 265-272.
10. Nemanič, V.; Žumer, M., Quantification of small gas amounts with an ion trap mass spectrometer, *International Journal of Mass Spectrometry* 2016, 401, 17-21

## Patents granted

1. Alenka Vesel, Miran Mozetič, Rok Zaplotnik, Device for high-frequency gas plasma excitation, DE112012000015 (B4), Deutsches Patent- und Markenamt, 21. 04. 2016
2. Alenka Vesel, Rok Zaplotnik, Miran Mozetič, Method for cleaning of with body fluid-contaminated medical implantants and devices with the use of atomic oxygen, SI24840 (A), Slovenian Intellectual Property Office, 29. 04. 2016
3. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič, A method of colouring titanium and titanium alloys, SI24851 (A), Slovenian Intellectual Property Office, 29. 04. 2016

## INTERNATIONAL PROJECTS

1. 7FP - IP4Plasma; Industrial Innovations Based on EU Intellectual Property Assets in the Field of Atmospheric Plasma Technology  
Asst. Prof. Janez Kovač  
European Commission
2. COST TD1208; Electrical Discharges with Liquids for Future Applications; COST Training School on Liquid Discharges  
Prof. Uroš Cvelbar  
Cost Office
3. NATO Grant; SPS 984555; Atmospheric Pressure Plasma Jet for Neutralisation of CBW  
Prof. Uroš Cvelbar  
Nato - North Atlantic Treaty Organisation
4. COST CA15114; Anti-Microbial Coating Innovations to prevent Infectious Diseases (AMICI)  
Prof. Uroš Cvelbar  
Cost Office
5. Education-ED-FU, EUROFUSION  
Prof. Miran Mozetič  
European Commission
6. Sniffing for Carcinogenic Substances - Research for Toxic Gas Molecule Sensing with Networks of Carbon Nanowalls  
Prof. Uroš Cvelbar  
Slovenian Research Agency
7. Advanced Photo-electrochemical Cells with Nanostructured Iron Oxide Electrodes  
Prof. Miran Mozetič  
Slovenian Research Agency
8. Irradiation of Metal Oxide Nanowires  
Prof. Uroš Cvelbar  
Slovenian Research Agency
9. Biocompatible Nanostructured Tetragonal Zirconium Oxide Thin Films with Alternative Stabilization Dopants  
Prof. Miran Mozetič  
Slovenian Research Agency
10. Innovative Method for Synthesis of Thin Absorption Films for Photovoltaics  
Asst. Prof. Alenka Vesel  
Slovenian Research Agency
11. Sterilization of Heat-sensitive Materials with Innovative Plasma Source of UV Radiation  
Prof. Miran Mozetič  
Slovenian Research Agency
12. Dust in Plasmas (DIP)  
Prof. Miran Mozetič  
Slovenian Research Agency
13. MS-MZDR/16-1-B2-071; ECS Electrochemical Society  
Prof. Uroš Cvelbar  
Slovenian Research Agency
14. Presentations and Invited Talk at the Conference at the University of Liverpool: Plasma Technology as a Tool for the Inactivation of Food-related Microorganisms  
Prof. Miran Mozetič  
Slovenian Research Agency
15. Small Services  
Prof. Uroš Cvelbar

## 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. Understanding plasma processes and thin film growth in High Power Impulse Magnetron Sputtering  
Prof. Uroš Cvelbar
2. Nanoscale engineering of the contact interfaces for green lubrication technology  
Asst. Prof. Janez Kovač
3. Multifunctional electrospun nanofibers development and dynamic interaction studies with pathogen bacteria  
Prof. Miran Mozetič
4. Development of the functional textiles used for the treatment of diabetic foot (malum perforans)  
Prof. Miran Mozetič
5. New materials for printed sensors and indicators and their integration in smart printed matter  
Asst. Prof. Alenka Vesel
6. Interaction between fully dissociated moderately ionized ammonia plasma and glass-fiber reinforced polymers  
Prof. Miran Mozetič
7. Nanostructures and related composites for detection of hazardous gaseous molecules  
Prof. Uroš Cvelbar
8. Functionalization of polymer cardiovascular implants for optimal hemocompatibility  
Asst. Prof. Alenka Vesel
9. New generation of superior creep resistant steels with nanoparticles modified microstructure  
Prof. Uroš Cvelbar
10. Advanced hydrodesulphurisation with catalyst nanomaterials  
Prof. Uroš Cvelbar
11. Advanced hemocompatible surfaces of vascular stents  
Dr. Ita Junkar
12. Self-lubricating and wear resistant PVD hard coatings based on (V,Cr,Al,Ti)N for hot-working processes  
Asst. Prof. Janez Kovač
13. Building blocks, tools and systems for the Factories of the Future - GOSTOP  
Prof. Miran Mozetič
14. Food for future - F4F  
Asst. Prof. Alenka Vesel
15. Potential of biomass for development of advanced materials and bio-based products  
Dr. Ita Junkar
16. Novel type of antibacterial coatings on textile materials and plastics with controllable release of antibacterial agent  
Prof. Uroš Cvelbar  
Hydrogen Permeation Measurements on PVD-Coated Eurofer  
Dr. Vincenc Nemanič  
Ústav Fyziky Plazmatu Av Čr, V. V. I.

## VISITORS FROM ABROAD

1. Prof. Dr Xiao Xia Zhong, Shanghai University, Shanghai, China, 31 January-1 February 2016
2. Prof. Dr Xiao Xia Zhong, Shanghai University, Shanghai, China, 10-12 February 2016
3. Prof. Dr Davide Mariotti, Ulster University, Jordanstown, UK, 2-5 April 2016
4. Prof. Dr Joanna Pawlat, Lublin University of Technology, Lublin, Poland, 16-17 April 2016
5. Prof. Dr Joanna Pawlat, University of Technology, Lublin, Poland, 21-22 April 2016
6. Prof. Stella W. Pang, The University of Hong Kong, Hong Kong, China, 15-17 May 2016
7. Prof. Lin Dai, The University of Hong Kong, Hong Kong, China, 15-17 May 2016
8. Prof. Rosa Chan, The University of Hong Kong, Hong Kong, China, 15-17 May 2016
9. Christian Nöbauer, Vienna University of Technology, Vienna, Austria, 22-26 May 2016
10. Yishan Han, Shanghai University, Shanghai, China, 5-14 June 2016
11. Prof. Jiang Yong Wang, Shanghai University, Shanghai, China, 9-14 July 2016
12. Doc. Ing. Petr Slobodian, Ph.D., Tomas Bata University in Zlín, Zlín, Czech Republic, 20-23 September 2016
13. Jiri Matyas, Tomas Bata University in Zlín, Zlín, Czech Republic, 20-23 September 2016
14. Ondra Grulich, Tomas Bata University in Zlín, Zlín, Czech Republic, 1 August-30 September 2016

15. Martina Minaříka, Tomas Bata University in Zlín, Zlín, Czech Republic, 1 August–30 September 2016
16. Prof. Dr Hyung Jun Cho, Nagoya University, Nagoya, Japan, 12–15 November 2016
17. Christian Nöbauer, Vienna University of Technology, Vienna, Austria, 20–22 October 2016
18. Prof. Dr Christoph Eisenmenger – Sittner, Vienna University of Technology, Vienna, Austria, 20–22 October 2016
19. Masakazu Tomatsu, Nagoya University, Nagoya, Japan, 12–15 November 2016
20. Prof. Dr Makota Sekine, Nagoya University, Nagoya, Japan, 12–15 November 2016
21. Prof. Dr Petr Špatenka, Czech Technical University in Prague, Prague, Czech Republic, 22–24 November 2016

## STAFF

### Researchers

1. Prof. Uroš Cvelbar
  2. *Dr. Aleksander Drenik, on leave 01.03.16*
  3. Dr. Ita Junkar
  4. Asst. Prof. Janez Kovač
  5. **Prof. Miran Mozetič, Head**
  6. Dr. Vincenc Nemanič
  7. Asst. Prof. Alenka Vesel
  8. Dr. Rok Zaplotnik
- Postdoctoral associates
9. Dr. Gregor Filipič
  10. *Dr. Gregor Jakša, left 01.09.16*
  11. Dr. Martina Modic

12. Dr. Gregor Primc
  13. Dr. Nina Recek
- Postgraduates
14. Nataša Hojnik, B. Sc.
  15. Matej Holc, B. Sc.
  16. Matic Resnik, B. Sc.
  17. Marko Žumer, B. Sc.
- Technical officers
18. Tatjana Filipič, B. Sc.
- Technical and administrative staff
19. Tinkara Bezovšek, B. Sc.
  20. Urška Kisovec, B. Sc.
  21. Janez Trtnik

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## SHORT ARTICLE

1. Mukta Vishwanath Kulkarni, Ita Junkar, Harinarayanan Puliyalil, Aleš Igljič, "Wettability switch of anodic titanium dioxide nanotubes with various diameters", *Biophys. j.*, vol. 110, iss. 3, sup. 1, pp. 339a, Feb. 2016.

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1. Somayeh Akbari, Janez Kovač, Mitjan Kalin, "Study the chemical structure of the ZDDP thermal film on steel and dlc surfaces at different times and ZDDP concentrations using ATR-FTIR and XPS", In: *Zbornik predavanj posvetovanja o tribologiji, mazivih in tehnični diagnostiki, SLOTRIB 2016*, f. 91-105.
2. Mojca Božič, Vera Vivod, Robert Vogrinčič, Silvo Hribernik, Irena Ban, Gregor Jakša, Darinka Fakin, Vanja Kokol, "New photocatalysts based on the surface modified TiO<sub>2</sub>-MWCNTs for decolourization of methylene blue dye", In: *Proceedings, 16th World Textile Conference AUTEX 2016, 8-10 June 2016, Ljubljana, Slovenia*, pp. 1-7.
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Ita Junkar, "Interaction of cells and platelets with biomaterial surface treated with gaseous plasma", In: *Advances in biomembranes and lipid self-assembly. Volume 23*, Aleš Iglič, ed., Chandrashekar Kulkarni, ed., Michael Rappolt, ed., Amsterdam [etc.], Elsevier, 2016, pp. 25-59.
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## PATENT

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2. Alenka Vesel, Rok Zaplotnik, Miran Mozetič, *Method for cleaning of with body fluid-contaminated medical implantants and devices with the use of atomic oxygen*, SI24840 (A), Urad RS za intelektualno lastnino, 29. 04. 2016.
3. Gregor Filipič, Kristina Eleršič, Darij Kreuh, Janez Kovač, Uroš Cvelbar, Miran Mozetič, *A method of colouring titanium and titanium alloys*, SI24851 (A), Urad RS za intelektualno lastnino, 29. 04. 2016.

## MENTORING

1. Harinarayanan Puliyalil, *Selective plasma etching of polymer matrix composites for improvement of their surface properties*: doctoral dissertation, Ljubljana, 2016 (mentor Uroš Cvelbar; co-mentor Miran Mozetič).

# 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 one side, 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 "Jozef Stefan Institute" is performed in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the J. Stefan International Postgraduate School. In 2016, the research was performed within three research programs:

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

## ***I. Program group "Magnetic resonance and dielectric spectroscopy of smart new materials"***

The research of the program group *Magnetic Resonance and Dielectric Spectroscopy of Smart New Materials* was focused on the 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 attained knowledge provides the key to the understanding of the microscopic and macroscopic properties of various types of solids and is an important condi-

**The research group has discovered new quantum phenomena in the magnetism of low-dimensional spin systems. It has studied physical properties of a novel type of nanomaterials suitable for gas sensors and has discovered new materials with a giant electrocaloric effect for applications in cooling devices. The group has developed new polymer-dispersed liquid-crystalline elastomers. The Schottky effect has been demonstrated in quasicrystals, which fundamentally changes the interpretation of their low-temperature electronic and magnetic properties. The research has included pharmaceutical and biological substances.**

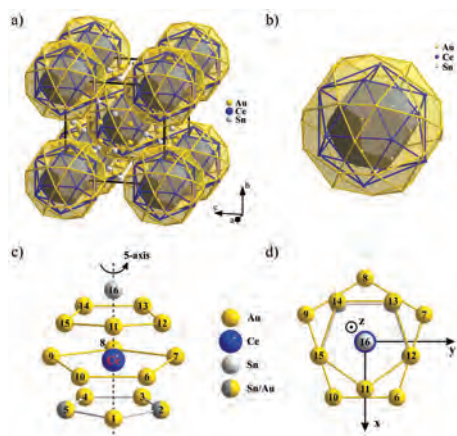


Figure 1: Icosahedral structure and pentagonal distribution of electric charges in Ce-Au-Sn-type quasicrystals for the calculation of the Schottky effect.

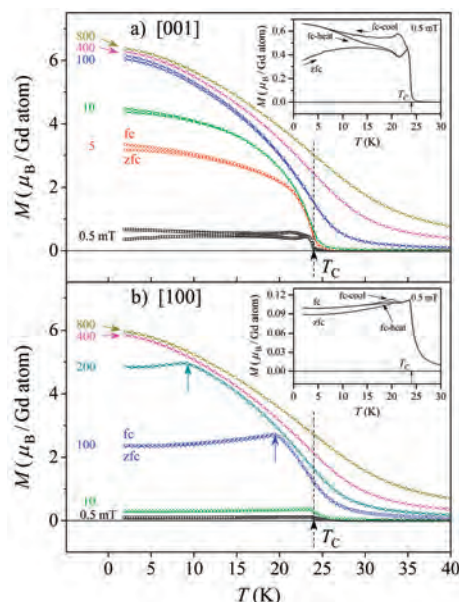


Figure 2: Temperature-dependent magnetization of the Cu-Ca-Gd alloy for a magnetic field directed along the hexagonal axis and in the hexagonal plane.

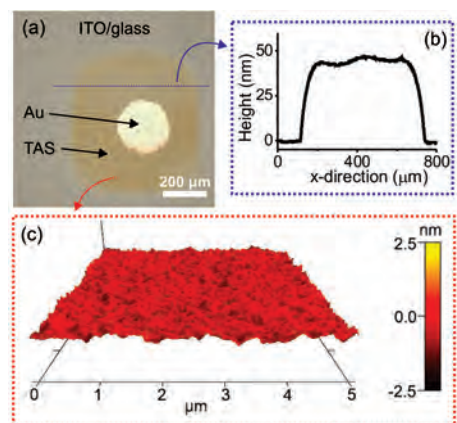


Figure 3: (a) Optical photograph, (b) cross-sectional profile, and (c) 3D AFM topology image of 45-nm-thick printed tantalum-oxide-based (TAS) thin-film capacitor.

tion for the discovery and development of new multifunctional materials and nanomaterials for novel technological applications.

The research program was implemented in close collaboration with the Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics, and the J. Stefan International Postgraduate School.

In 2016, members of the program group published 47 original scientific papers in international peer-reviewed scientific journals. Among these, one paper was published in *Nature Commun.* (IF = 11.3), one in *Phys. Rev. Lett.* (IF = 7.6), one in *ACS Applied Mater. & Interfaces* (IF = 7.1), two in *Sci. Rep.* (IF = 5.2), and three in *J. Mater. Chem. C* (IF = 5.1).

The investigations were focused on the following research fields:

### Quasicrystals and complex metallic alloys

In the publication *Schottky effect in the i-Zn-Ag-Sc-Tm icosahedral quasicrystal and its 1/1 Zn-Sc-Tm approximant* (S. Jazbec et al., *Phys. Rev. B* 93, 054208 (2016)) we have for the first time experimentally proved the existence of the Schottky effect in quasicrystals. This discovery fundamentally changes the current interpretations of the low-temperature electronic and magnetic effects in quasicrystals and their periodic approximants. We have developed the theory of the Schottky effect for the pentagonal symmetry of the crystal electric fields, applicable to quasicrystals of the structural type Ce-Au-Sn. The icosahedral structure and pentagonal distribution of electric charges in Ce-Au-Sn are shown in Figure 1.

In the publication *Random-anisotropy ferromagnetic state in the Cu<sub>5</sub>Gd<sub>0.54</sub>Ca<sub>0.42</sub> intermetallic compound* (M. Krnel et al., *Phys. Rev. B* 93, 094202 (2016)) we presented the synthesis of the first ternary compound in the Cu-Ca-Gd system, where the immiscible elements Ca and Gd are chemically bound into a crystal by the third “intervening” element copper, which makes stable binary phases with both elements. We determined physical properties for this new ternary alloy and showed that its magnetic state can be described as a random-anisotropy ferromagnet. Figure 2 shows the temperature-dependent magnetization of the alloy for a magnetic field directed along the hexagonal axis and in the hexagonal plane.

### Inkjet printing of uniform dielectric oxide structures

Inkjet printing of high-dielectric-constant metal-oxide layers will enable the low-cost deposition of the essential building blocks in electronics. We have developed an ink formulation suitable for the printing of tantalum-oxide-based dielectric layers. Our goal was to improve the thickness uniformity of dried deposits via optimization of the ink’s solvent composition. We have shown that in addition to designing the solvent mixture according to the viscosity and surface-tension criteria, the volatility of solvents has to be considered, as it strongly influences the thickness uniformity. By rigorously adjusting the solvent composition, we were able to tailor the topology of the deposits and print 45-nm-thick, flat and uniform capacitors with functional properties comparable to spin-coated films. We published our discoveries in *Inkjet printing of uniform dielectric oxide structures from sol-gel inks by adjusting the solvent composition* (A. Mataž, R. C. Frunz, A. Drnovšek, V. Bobnar, B. Malič, *Journal of Materials Chemistry C* 4, 5634 (2016)).

### Development of an eco-friendly material for flexible energy-storage devices

Nanocomposite films were fabricated by incorporating ammonia-functionalized graphene oxide (NGO) into the native (CNF) and TEMPO-oxidized (TCNF) cellulose nanofibrils matrices using a solvent-casting method. The structural and morphological analysis revealed good dispersibility of the NGO sheets in the randomly distributed CNF, and the dense and parallel-oriented TCNF nanofibrils. Such a synergistic effect of both components contributed to ultra-strong and stiff films with good mechanical and thermal stability. Due to the Maxwell-Wagner polarization, the dielectric constant strongly increases already at a low NGO content. Thus, this mechanically strong, flexible, and thermally stable composites are suitable, cost-effective, alternative green materials for flexible energy-storage devices. This research was published in the paper *Mechanically strong, flexible and thermally stable graphene oxide/nanocellulosic films with enhanced dielectric properties* (Y. Beeran P. T. et al., *RSC Advances* 6, 49138 (2016)).

### Stable dielectric response of newly developed low-loss polymer thin films

We have investigated the dielectric properties of aromatic polythiourea (ArPTU, polar polymer

containing high dipolar moments with very low defect levels) thin films that were developed on a Pt/SiO<sub>2</sub> substrate. The detected response was compared to the response of commercially available polymers, such as high-density polyethylene (HDPE) and polypropylene (PP), which are at the present both used in foil capacitors. Stable values of the dielectric constant (being two times higher than in HDPE and PP) over broad temperature and frequency ranges and dielectric losses as low as in commercial systems suggest that ArPTU is a promising candidate for future use in a variety of applications. The findings were published in *Stable dielectric response of low-loss aromatic polythiourea thin films on Pt/SiO<sub>2</sub> substrate* (A. Eršte et al., Journal of Advanced Dielectrics 6, 1650003 (2016)).

#### Study of nanostructured materials and materials with large electrocaloric effect and its application in a solid-state cooling device:

Using direct measurements, we showed the coexistence of both the electrocaloric and magnetocaloric effect in multiferroic PFN-PMW. We were among the first to demonstrate the existence of a large electrocaloric effect in liquid crystals and of a large elastocaloric effect in liquid-crystal elastomers. In addition, we have analysed the working cycle of a prototype of a cascade electrocaloric device exploiting both the electrocaloric and electromechanic effects. In 2016, the Gorenje d.d. company bought our *Patent application US 2016/0187034 A17700*, 2016, (B. Malič et al.). The above results were published in 11 articles in international scientific journals, among which we must mention *Perovskite ferroelectrics and relaxor-ferroelectric solid solutions with large intrinsic electrocaloric response over broad temperature ranges* (H. Khassaf et al., P. Journal of Materials Chemistry C, 4 (2016), 4763), *A multicaloric material as a link between electrocaloric and magnetocaloric refrigeration* (H. Uršič et al., Scientific Reports, 6 (2016), 26629-1-26629-5), *BaZr<sub>0.5</sub>Ti<sub>0.5</sub>O<sub>3</sub>: Lead-free relaxor ferroelectric or dipolar glass* (C. Filipič, Z. Kutnjak, R. Pirc, G. Canu, J. Petzelt, Physical Review B, 93 (2016), 224105-1-224105-8), and *Electrocaloric and elastocaloric effects in soft materials* (M. Trček et al., Philosophical Transactions A, 374 (2016), 20150301). Recent publications on electrocalorics and TGB and blue phases have been cited more than 100 times in 2016.

#### Nanomaterials for gas-sensor applications

Polona Umek collaborated with colleagues from Great Britain, Czech Republic, Belgium, France and Spain in the research of gas sensors based on WO<sub>3</sub> nanoneedles (NN) decorated with PdO nanoparticles (NP). Morphological, structural, and elemental composition analysis revealed that a Pd(acac)<sub>2</sub> precursor was very suitable to decorate WO<sub>3</sub> NNs with uniform and well-dispersed PdO NPs. Gas-sensing results revealed that the decoration with PdO NPs led to an ultrasensitive and selective hydrogen (H<sub>2</sub>) gas sensor with a low operating temperature (150 °C). The response of the decorated NNs is 755-times higher than that of bare WO<sub>3</sub> NNs. Humidity measurements showed that PdO/WO<sub>3</sub> sensors displayed low-cross-sensitivity towards water vapour, compared to bare WO<sub>3</sub> sensors. The addition of PdO NPs helps to minimize the effect of ambient humidity on the sensor response. The research was published in the article *Aerosol-assisted CVD-grown PdO nanoparticle-decorated tungsten oxide nanoneedles extremely sensitive and selective to hydrogen* (F. E. Annanouch et al., ACS Applied Materials & Interfaces 8, 10413 (2016)).

#### Pharmaceutical substances studied by NQR spectroscopy

<sup>14</sup>N NQR is a useful tool to characterize pharmaceutical substances and the method of their preparation. In combination with other experimental techniques and quantum chemical calculations, the electronic structure of these molecules and the properties of functional groups can be determined, as shown in the article *Polymorphism and Thermal Stability of Natural Active Ingredients. 3,3'-Diindolylmethane (Chemopreventive and Chemotherapeutic) Studied by a Combined X-Ray, <sup>1</sup>H - <sup>14</sup>N NMR NQR, DSC and Solid-State DFT/3D HS/QTAIM/RDS Computational Approach* (J. N. Latosinska, M. Latosinska, M. Szafranski, J. Seliger, V. Žagar, Cryst. Growth Des. 16, 4336-4348 (2016)).

The compound 3,3'-diindolylmethane (DIM) is a major in-vivo product of the digestion of indole-3-carbinol (I3C) and a main mediator of its chemopreventive and chemotherapeutic effects. In this paper, the co-influence of two factors, polymorphism and temperature, on the topology, nature, and strength of the interaction pattern in DIM are in our area of interest. Upon polymorph screening, it has been found that DIM crystallizes in two polymorphic forms, form I (already known) and form II (newly obtained). Differential scanning calorimetry indicated a slightly lower melting point for form I than for

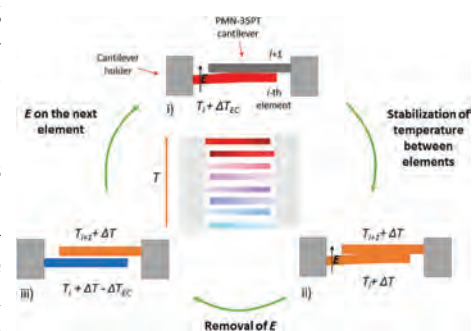


Figure 4: Schematics of the refrigeration cycle of cascade electrocaloric cooling device exploiting in cantilever cooling elements both an electrocaloric and electromechanic response.

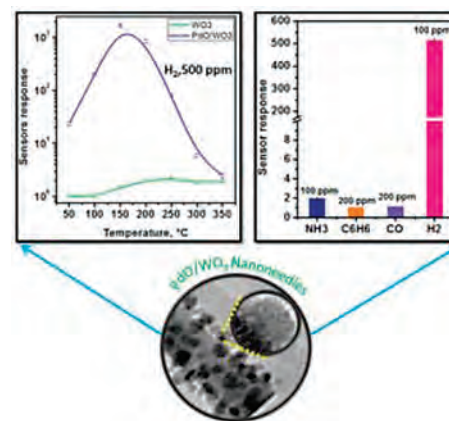


Figure 5: Left: sensor response (WO<sub>3</sub> nanoneedles decorated with PdO nanoparticles) on 500 ppm of H<sub>2</sub> between 50 and 350 °C (violet curve) compared with a sensor based on bare WO<sub>3</sub> nanoneedles (green curve). Right: Selectivity diagram of PdO/WO<sub>3</sub> sensor toward NH<sub>3</sub>, C<sub>6</sub>H<sub>6</sub> and CO interfering gases.

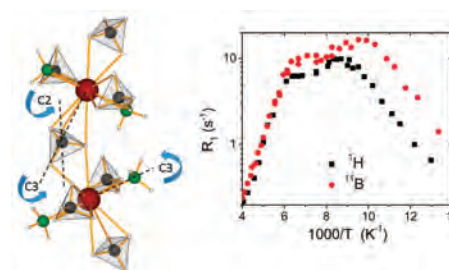


Figure 6: <sup>1</sup>H NMR relaxometric study of molecular dynamics in a "de Vries" liquid crystal.



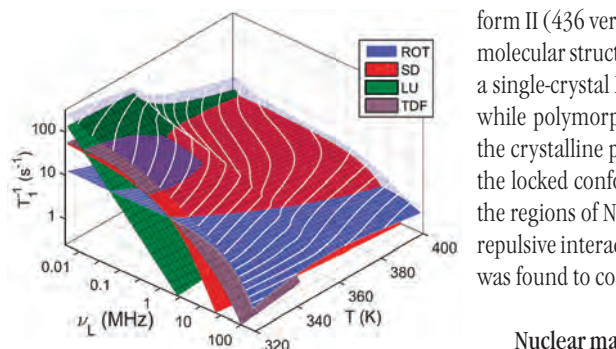


Figure 7.  $^1\text{H}$ - $^{14}\text{N}$  cross-relaxation spectrum analysis in sildenafil and sildenafil citrate.

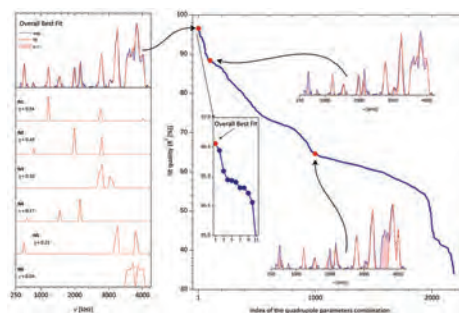


Figure 8. Left: Sildenafil  $^1\text{H}$ - $^{14}\text{N}$  CR spectrum: the experimental data (solid blue line) and the overall best fit (solid red line). A decomposition of the best fit in contributions from individual nitrogen sites is also shown. Right: The quality of sildenafil CR spectrum fits for all combinations of transition pairing. Here two spectra with poor fits are also shown.

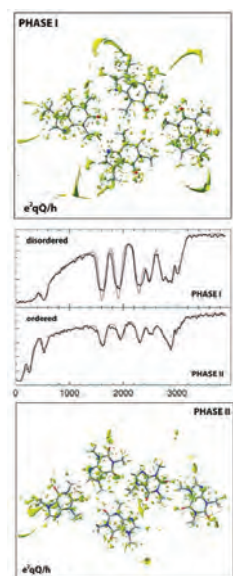


Figure 9: Isosurface plot of EFG asymmetry parameter at each point of the molecular system for phase I (top) and phase II (bottom) of caffeine. Cross-relaxation spectra of caffeine in both phases are shown in the middle.

form II (436 versus 440 K) and the lack of phase transitions in both polymorphs. The crystal and molecular structures of both polymorphs have been determined as a function of temperature from a single-crystal X-ray diffraction. The structure of polymorph I is monoclinic, space group  $C2/c$ , while polymorph II is orthorhombic, space group  $P2_12_12_1$ . The key interaction that determines the crystalline packing in both polymorphs of DIM is the  $\text{NH}\cdots\pi$  one. The factor responsible for the locked conformation of DIM in both forms is the electrostatic potential complementarity of the regions of  $\text{N}-\text{H}\cdots\pi$ , linking neighbouring molecules, which permits easy overcoming of any repulsive interactions that may force the rotation of the molecule. The commercial sample of DIM was found to contain approximately 50% of form I and 50% of form II.

### Nuclear magnetic resonance study of molecular dynamics in ammine metal borohydride $\text{Sr}(\text{BH}_4)_2(\text{NH}_3)_2$

Borohydrides are promising hydrogen-storage materials due to their high hydrogen content and relatively low decomposition temperature. In the article *Nuclear magnetic resonance study of molecular dynamics in ammine metal borohydride  $\text{Sr}(\text{BH}_4)_2(\text{NH}_3)_2$*  (A. Gradišek, L. H. Jepsen, T. R. Jensen, M. S. Conradi, *J. Phys. Chem. C*, 2016, 120, 24646-24654), we investigated  $\text{Sr}(\text{BH}_4)_2(\text{NH}_3)_2$ , a novel system that contains hydrogen in two molecular groups -  $\text{BH}_4$  and  $\text{NH}_3$ . Molecular dynamics was studied by means of  $^1\text{H}$  and  $^{11}\text{B}$  NMR spectra and spin-lattice relaxation. We identified activation energies for the rotations of  $\text{BH}_4$  tetrahedra around two different symmetry axes. Low-temperature measurements unveiled that there are some motions still present around 4 K. In addition, we studied a partially deuterated modification of the compound to further distinguish dynamic processes.

Liquid crystals that exhibit *de Vries* smectic A phases are promising materials for new generations of ferroelectric liquid-crystal displays and other electro-optical devices. We investigated the molecular dynamic properties of a rod-like *de Vries* liquid-crystal compound in the whole mesophasic range by means of fast field-cycling NMR relaxometry. The main molecular motions, i.e., reorientational diffusion, translational self-diffusion, layer undulation, and tilting director fluctuations were fully characterized. The molecular dynamics' behaviour observed across the  $\text{SmA}-\text{SmC}^*$  phase transitions of 9HL was consistent with the proposed *cluster diffuse cone* model for the *de Vries*  $\text{SmA}$  phase. The findings were published in the article  *$^1\text{H}$  NMR relaxometric study of molecular dynamics in a "de Vries" liquid crystal* (A. Gradišek, V. Domenici, T. Apih, V. Novotná, P. J. Sebastião, *J. Phys. Chem. B*, 2016, 120, 4706-4714).

$^1\text{H}$ - $^{14}\text{N}$  cross-relaxation (CR) spectroscopy is a powerful technique to determine  $^{14}\text{N}$  NQR parameters ( $C_q^-$ ), as it requires very small quantities of material. However, the NQR parameters cannot be determined directly from the CR spectrum, but rather through an intermediate step called "peak pairing", that is, finding pairs of  $^{14}\text{N}$  transitions belonging to the same nitrogen site. "Peak pairing" is far from straightforward and typically requires good intuition. In order to facilitate CR spectra analysis and make the procedure more robust, we developed an automatic method, which simultaneously fits the lineshapes for all the  $^{14}\text{N}$  transitions for all possible combinations of transition pairs, where finally we choose the combination with an overall best fit of the spectrum. For substances with several nitrogen sites, there may be thousands of pairing combinations, but nevertheless, the automatic procedure is still significantly faster than the manual "peak pairing". We have demonstrated the technique on sildenafil (Figure 8) and sildenafil citrate, which both have six nitrogen sites, and published the results in the article  *$^1\text{H}$ - $^{14}\text{N}$  cross-relaxation spectrum analysis in sildenafil and sildenafil citrate* (A. Gregorovič, T. Apih, J. Seliger, *Solid State Nuc. Mag.* 78, 16 (2016)).

### Polymorphism of caffeine

The polymorphism of anhydrous caffeine has been studied by  $^1\text{H}$ - $^{14}\text{N}$  NMR-NQR (Nuclear Magnetic Resonance-Nuclear Quadrupole Resonance) double resonance and pure  $^{14}\text{N}$  NQR (Nuclear Quadrupole Resonance) and by computational modelling (Density Functional Theory) in the solid state. The assignment of NQR signals detected in stable phase I and in metastable phase II to particular nitrogen sites was verified with the help of DFT. The commercial pharmaceutical sample was found to contain approximately 20–25% of phase I and 75–80% of phase II. The orientational disorder in phase II with a local molecular arrangement mimics that in phase I. Substantial differences in the intermolecular interaction phases I and II of caffeine were analysed using a computational (DFT/QTAIM/RDS) approach and the maps of the principal component of the EFG tensor and its asymmetry parameter at each point of the molecular system were calculated and visualized. The relevant maps calculated for both phases I and II indicate a small variation in electrostatic potential upon phase change. These small differences between packings in phases only slightly disturb the neighbourhood of the N(1) and N(7) nitrogens, and are thus meaningless

from the biological point of view. The composition of the two phases in pharmaceutical material should not be an obstacle, which is relevant from the point of view of the pharmaceutical industry.

The study was published in the article *Polymorphism and disorder in natural active ingredients. Low and high-temperature phases of anhydrous caffeine: Spectroscopic ( $1H$ - $14N$  NMR-NQR/ $14N$  NQR) and solid-state computational modelling (DFT/QTAIM/RDS) study* (J. Seliger et al., European Journal of Pharmaceutical Sciences, 85 (2016), 18).

### Polymer-dispersed liquid-crystal elastomers

We have experimentally investigated the orientational ordering of thermomechanically active liquid-crystal elastomer microparticles dispersed in a PDMS elastomer, using quadrupole-perturbed deuteron NMR. We have also developed a theoretical model of the behaviour of orientational order parameter  $Q$  in the external magnetic field  $B$  as a function of the microdomain nematic order parameter  $S$  and diamagnetic anisotropy  $\Delta\mu$ , the viscosity of the uncured matrix resin  $\eta$ , and of the curing process kinetic factor  $k$ . By comparing theoretical predictions with the experimentally determined values of  $Q(B)$ , we have demonstrated that the degree of orientational ordering and, consequently, the effective thermomechanical response of the composite material can be tailored by controlling the external magnetic field as well as by properly adjusting the curing time. The research on polymer-dispersed liquid crystal was published in two articles: *Deuteron NMR resolved mesogen vs. crosslinker molecular order and reorientational exchange in liquid single crystal elastomers* (J. Milavec, V. Domenici, B. Zupančič, A. Rešetič, A. Bubnov in B. Zalar, Physical Chemistry Chemical Physics 18, 4071-4077 (2016)) and *Polymer-dispersed liquid crystal elastomers*, (A. Rešetič, J. Milavec, B. Zupančič, V. Domenici in B. Zalar, Nature Communications 7, 13140 (2016)).

### Quantum magnetism

Matej Pregelj, Matjaž Gomilšek, Andrej Zorko, and Denis Arčon, in collaboration with partners from Switzerland, Croatia and France, investigated the mechanism responsible for the occurrence of an unusual spin-stripe phase in the  $\beta$ -TeVO<sub>4</sub> compound, which represents a model system of the frustrated ferromagnetic spin-1/2 chain. A combination of magnetic-torque, neutron-diffraction, and spherical-neutron-polarimetry measurements was employed to determine all the magnetic structures that the system develops on cooling in the absence of a magnetic field, i.e., in the vectorchiral phase, in the spin-stripe phase and in the collinear amplitude-modulated phase. Based on these results, they developed a phenomenological model that revealed the anisotropy of the exchange interaction as the key ingredient for the spin-stripe formation in frustrated spin systems. Their discovery was published in the article *Exchange anisotropy as mechanism for spin-stripe formation in frustrated spin chains* (M. Pregelj et al., Phys. Rev. B 94, 081114(R) (2016)).

Matjaž Gomilšek, Martin Klanjšek, Matej Pregelj, and Andrej Zorko collaborated with researchers from China, United Kingdom, and Switzerland in an in-depth investigation of magnetic properties of Zn-brochantite. This is a new realization of the quantum kagome antiferromagnet, a paradigm of geometrical frustration in two dimensions, that was synthesized by the Chinese collaborators in 2014. With the use of various experimental techniques, including nuclear magnetic resonance, muon spin relaxation/rotation, and neutron scattering they established that the ground state of this material is magnetically disordered and dynamical. They observed a quantum-critical behaviour at high temperatures and various spin-liquid instabilities that the system goes through with lowering temperature. Their discovery was published in the paper *Instabilities of spin-liquid states in a quantum kagome antiferromagnet* (M. Gomilšek et al., Phys. Rev. B 93, 060405(R) (2016)).

Additionally, they showed that the low-temperature spin-liquid phase behaves like a spinon metal, which is a novel type of behaviour for the kagome lattice. This observation was published in the paper  *$\mu$ SR insight into the impurity problem in quantum kagome antiferromagnets* (M. Gomilšek et al., Phys. Rev. B 94, 024438 (2016)).

Andrej Zorko, Matjaž Gomilšek, and Matej Pregelj, in collaboration with researchers from Germany, USA, Moldova, and Switzerland investigated new functionality of layered metamagnets, with the use of electron spin resonance in high magnetic fields. The properties of the mixed antiferromagnetic/ferromagnetic phase that is stabilized in a finite range of applied fields around 0.8 T at low temperatures and is characterized by enhanced microwave absorption were thoroughly investigated. They showed that thermal fluctuations play an important role in destabilizing the

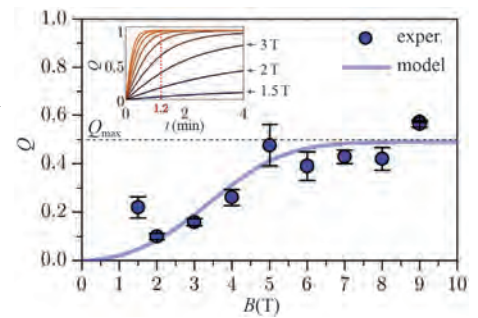


Figure 10: Orientational order parameter  $Q$  of liquid-crystal elastomer microparticles dispersed in a PDMS elastomer.  $Q$  saturates at  $Q_{\max} \approx 0.5$  for magnetic fields  $B \geq 5$  T.  $Q_{\max} < 1$  indicates that microparticles are not ideal nematic monodomains. The inset shows theoretically modelled time-dependence of the orientational ordering for different values of magnetic field, corresponding to experimental points  $Q(B)$  (blue circles).

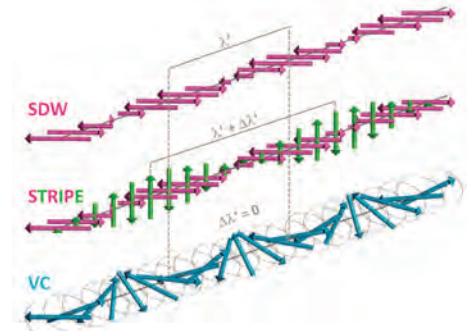


Figure 11: Magnetic order at the  $V_1$  site along the  $c$  axis derived for the collinear amplitude-modulated (SDW) phase, for the vector-chiral (VC) phase, and for the spin-stripe (STRIPE) phase.  $\lambda'$  corresponds to the deviation of  $k$  from  $1/2$ , i.e., from the antiferromagnetic modulation, while  $\Delta\lambda'$  corresponds to  $\Delta k$ . Published in M. Pregelj et al., Phys. Rev. B 94, 081114(R) (2016).

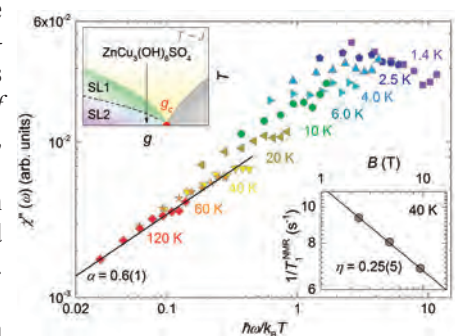


Figure 12: The observation of a quantum-critical scaling of the dynamical susceptibility in Zn-brochantite and the various magnetic states that the system goes through when lowering the temperature (upper inset). Published in M. Gomilšek et al., Phys. Rev. B 93, 060405(R) (2016).

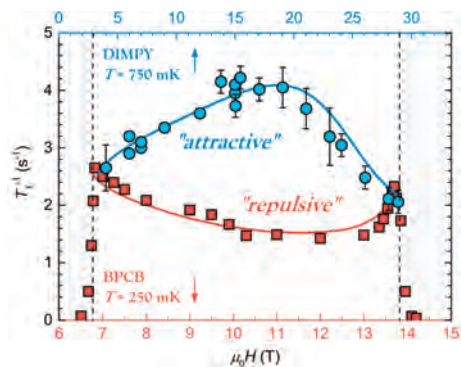


Figure 13: The observed difference of magnetic fluctuations probed by measurements of the spin-lattice relaxation time  $T_1$  in the systems BPCB and DIMPY, containing spin-1/2 ladders with strong rungs and strong legs, respectively.

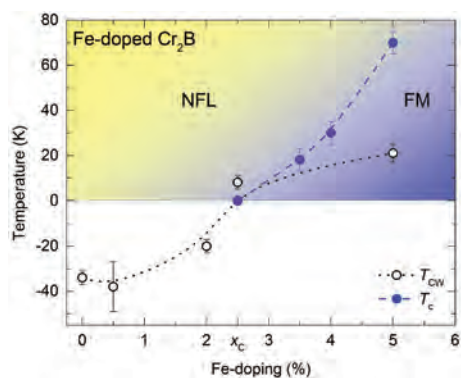


Figure 14: Phase diagram of Fe-doped  $\text{Cr}_2\text{B}$  system obtained from  $^{11}\text{B}$  NMR measurements.

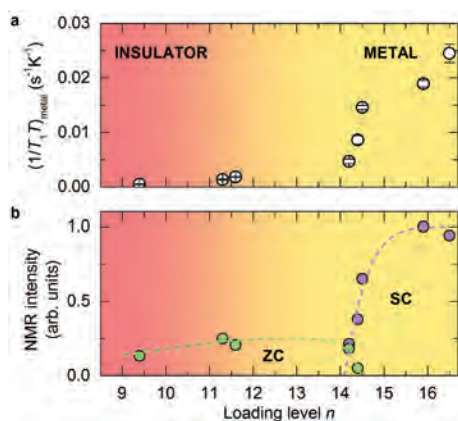


Figure 15: Phase diagram of the sodium-doped LSX zeolite showing the values of (a) metallic contribution to spin-lattice relaxation rate divided by temperature that is proportional to the square of electronic density-of-states, and (b) NMR spectrum intensity for shifted (SC) and unshifted (ZC) components as a function of Na loading level. The colour gradient divides the insulating and metallic regions.

highly absorbing mixed phase. Their discovery was published in the paper *Electron spin resonance insight into broadband absorption of the  $\text{Cu}_3\text{Bi}(\text{SeO}_3)_2\text{O}_2\text{Br}$  metamagnet*, (A. Zorko et al., AIP Advances 6, 056210 (2016)).

Andrej Zorko collaborated with researchers from France, USA and Switzerland in an in-depth neutron scattering investigation of magnetically and structurally chiral Fe langasite, which is a model system of triangle-based frustrated magnets with a strong potential for multiferroicity. They observed bunching of the helical modulation along the  $c$  axis and the in-plane distortion of the  $120^\circ$  Fe-spin arrangement. These observations enabled a refinement of the spin Hamiltonian, thus providing a link to the magnetically induced electric polarization observed in these systems. The results of this investigation were published in the paper *Helical bunching and symmetry lowering inducing multiferroicity in Fe langasites* (L. Chaix et al., Phys. Rev. B 93, 214419 (2016)).

Martin Klanjšek in collaboration with French and Swiss colleagues studied a difference in the magnetic response of the systems  $(\text{C}_5\text{H}_{12}\text{N})_2\text{CuBr}_4$  (BPCB) and  $(\text{C}_7\text{H}_{10}\text{N})_2\text{CuBr}_4$  (DIMPY), both containing the spin-1/2 ladders, where the exchange interactions along the rungs are stronger than those along the legs in the first case, and conversely in the second case. They confirmed that the spin ladders in both cases behave as a Tomonaga-Luttinger liquid of spinons. Nevertheless, the systems exhibit markedly different magnetic fluctuations, which can be directly probed by measurements of the spin-lattice relaxation time  $T_1$  in nuclear magnetic resonance. The observed difference emerges from the difference of interactions between the spinons in both cases: these are expectedly repulsive in the first case and surprisingly attractive in the second case. The work is published in *Dichotomy between Attractive and Repulsive Tomonaga-Luttinger Liquids in Spin Ladders* (M. Jeong et al., Phys. Rev. Lett. 117, 106402 (2016)).

Denis Arčon collaborated with groups from USA (Princeton University, University of Houston) and Israel (The Hebrew University of Jerusalem) on the evolution of magnetic fluctuations in systems, where we induce a transition between the paramagnetic and ferromagnetic metal using some external parameter (e.g., doping or pressure). Theoretical models in such cases predict the closeness of the quantum critical point (QCP) and strong deviations from the Fermi liquid behaviour. The research focused on two model systems, i.e., Fe-doped  $\text{Cr}_2\text{B}$  and  $\text{YFe}_2(\text{Ge},\text{Si})_2$ . In the former case we used  $^{11}\text{B}$  nuclear magnetic resonance data to discover the presence of both ferromagnetic and antiferromagnetic fluctuations. The latter are suppressed with Fe doping, before the ferromagnetic ones finally prevail for  $x > x_c$ . Indications for non-Fermi-liquid behaviour, usually associated with the proximity of a quantum critical point, were found for all samples, including undoped  $\text{Cr}_2\text{B}$ . The sharpness of the ferromagnetic-like transition changes on moving away from  $x_c$ , indicating significant changes in the nature of the magnetic transitions in the vicinity of the quantum critical point. Our data provided some important constraints for understanding quantum phase transitions in itinerant ferromagnets in the limit of weak quenched disorder. The results were published in *Evolution of magnetic fluctuations through the Fe-induced paramagnetic to ferromagnetic transition in  $\text{Cr}_2\text{B}$*  (D. Arčon et al., Phys. Rev. B 93, 104413 (2016)). The research of the  $\text{YFe}_2(\text{Ge},\text{Si})_2$  system had similar goals. The additional importance of these experiments lies in the fact that these structures are isostructural to some iron-based superconductors. We used  $^{89}\text{Y}$  NMR to show the presence of ferromagnetic fluctuations, which may have an impact on our understanding of the formation of Cooper pairs in this and other related compounds. The article was submitted to Phys. Rev. Lett. (J. Srpčič et al., arXiv:1608.01130 (2016)).

### Zeolites

Peter Jeglič and Denis Arčon, in collaboration with researchers from Slovenia and Japan, studied Na-type low-silica X (LSX) zeolite loaded with guest Na atoms. They unambiguously confirmed a metallic ground state for higher loading levels. By extracting the density-of-states at the Fermi level as a function of the sodium loading level, they discovered a continuous (crossover-like) evolution across the metal-to-insulator transition. These results reveal a complex loading-level dependence of electronic correlations and disorder due to electron confinement to zeolite cages and were published in the paper, *Metal-to-insulator crossover in alkali doped zeolite* (M. Igarashi et al., Sci. Rep. 6, 18682 (2016)).

## 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 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.

### Topology of liquid crystals: Singular points, skyrmions and torons

Chiral nematic liquid crystals exhibit rich topological phenomena, which were predicted and partially observed in chiral nematic droplets and thin liquid-crystal layers on patterned surfaces. It has been predicted that knots and links are stable in chiral nematic droplets, but this was difficult to observe because of the lack of appropriate experimental methods. We have developed a new method for the reconstruction of the director field, which is based on Fluorescent Confocal Polarisation Microscopy (FCPM) imaging in low birefringent liquid crystals with added fluorescent dyes. A new approach was taken in reconstructing the director field in chiral nematic droplets based on a simulated annealing algorithm. This combined method proved to be very efficient in reconstructing experimental 3D FCMP images. We observed that in chiral nematic droplets, topological singularities always appear in a form of point defects or simple rings, which are never knotted or linked. The complexity of the topological structures in chiral nematic droplets depends on the ratio of the helical pitch of the liquid crystal and the diameter of the droplet. In the case of low chirality, the number of point defects is small and they tend to be expelled to the surface of the droplet. The number of defects is always odd, which is due to the conservation of the total topological charge. We successfully reconstructed droplet structure with three point defects, which showed a cross-section of the Bloch skyrmion, which is similar to skyrmion structures in chiral magnets. When the number of point defects is increased to five for higher chirality, we observed another topological structure, which is akin to the toron structure observed in thin chiral nematic layers. Both skyrmion and toron structures are smoothly embedded in spherical confinement. This work presents the first exact reconstruction of the topology of 3D director in chiral nematic droplets and was published in *Scientific Reports* (G. Posnjak, S. Čopar and I. Muševič, *Scientific Reports* 6: 26361 (2016)).

Skyrmion structures were also observed in thin nematic LC films on chemically patterned patchy surfaces. When the sample was quenched from the fully aligned state using a strong external electric field, the director on the patterned patches spontaneously relaxed into a vortex-like structure, centred on the patch, as shown in the crossed-polarised image in Figure 17. This work was published in Cattaneo et al., *Soft Matter* 12, 853 (2016).

### Sensing surface morphology of biofibers by decorating spider silk and cellulosic filaments with nematic microdroplets

Liquid-crystal droplets deposited on microthin biofibres – including spider silk and cellulosic fibres – were shown to reveal characteristics of the fibres’ surface, performing as simple but sensitive surface sensors. By combining experiments and numerical modelling, different types of fibres are identified through the fibre-to-nematic droplet interactions, including perpendicular and axial or helicoidal planar molecular alignment. The nematic droplets as sensors also directly reveal the chirality of the cellulosic fibres. Different fibre entanglements can be identified by depositing droplets exactly at the fibres’ crossings. More generally, the presented method can be used as a simple but powerful approach for probing the surface properties of small-size bio-objects, opening a route to their precise characterization. This work is a collaboration between the soft matter

**The group explored topological defects in liquid-crystal droplets and shells, the structure of droplets on biofibres and in defect annihilation in liquid crystals. We developed super-resolution microscopy based on microlaser particles and biodegradable optical waveguides for photomedicine. We explored the working mechanism of the motor protein kinesin-14, new low-friction and low-dimensional nanomaterials.**

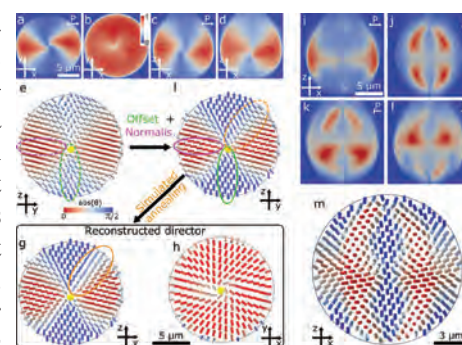


Figure 16: (a-d, i-l) Examples of fluorescent images taken at different polarisations of the fluorescent excitation beam. The panels (e-m) show the reconstructed director structure in a chiral nematic droplet.

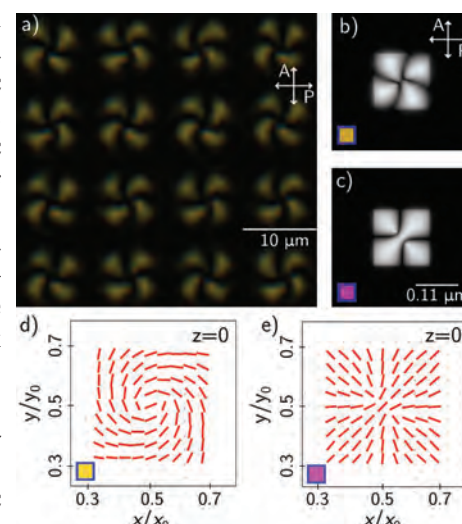


Figure 17: Skyrmions are vortex-like structures, which are clearly observed between crossed polarisers. (a) Experimental optical microscopy image viewed in white light transmission between crossed polarizers after the application of a potential of 30 V. (b and c) Are simulated optical microscopy images for two defect states with the lowest free energy; (d and e) are the corresponding director fields at the patterned surface ( $z = 0$ ).

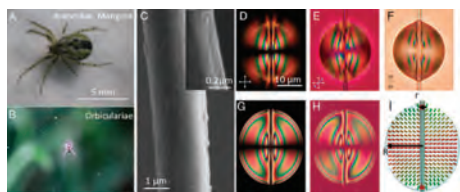


Figure 18: Droplets of a complex nematic fluid were shown to perform as robust sensors for detecting the surface morphology of bio-fibres, such as spider silk and cellulose (PNAS 113, 1174 (2016)).

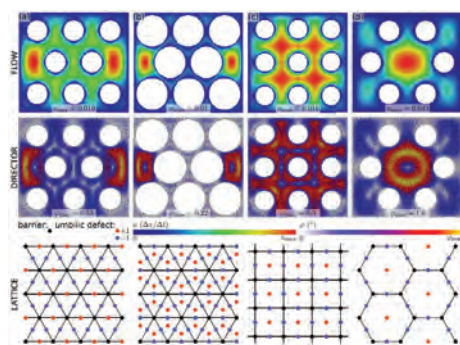


Figure 19: Porous nematic microchannels as generators of umbilic defect lattices (PRF 1, 023303 (2016)).



Figure 20: During the fast quenching of a liquid crystal from isotropic to nematic phase tangle of defect lines appear (a) and two pairs of Saturn rings and anti-rings are formed around the glass fibre (c).

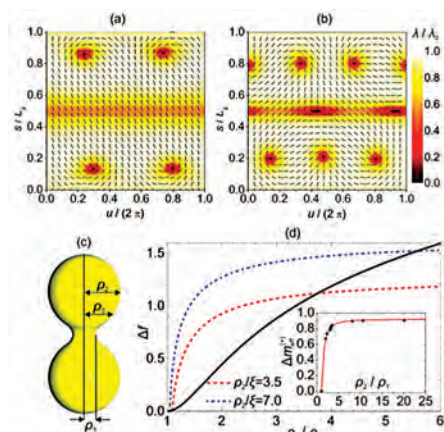


Figure 21: Depinning threshold in dumb-bell configurations. Panels (a, b) show nematic ordering in the  $(u, s)$  plane just below and above the threshold. The shape, calculated at the threshold, is presented in panel (c). In panel (d) the free-energy penalties to form a pair defect-antidefect and the effective topological charge are plotted as a function of geometrical parameters.

group in Ljubljana (modelling) and Lisbon (experiments) and was published in L. E. Aguirre et al., *Sensing surface morphology of biofibers by decorating spider silk and cellulosic filaments with nematic microdroplets*, Proc. Natl. Acad. Sci. USA 113, 1174 (2016).

### Porous nematic microfluidics for the generation of defect lattices as photonic crystals

Porous nematic microfluidics was demonstrated as a novel route for controlling the microstructure of the nematic order. Specifically, we showed the emergence of regular networks of topological defects, ranging in symmetry from triangular, square, to even kagome. This approach shows interesting possibilities as flow-tunable photonic crystal. The work was published in *Porous nematic microfluidics for generation of umbilic defects and umbilic defect lattices* (J. Aplinc, S. Morris and M. Ravnik, Phys. Rev. Fluids 1, 023303 (2016)).

### Annihilation dynamics of topological monopoles on a fibre in a nematic liquid crystal

We studied the dynamics of topological defects on a glass fibre immersed in a nematic liquid crystal. We have used the laser tweezers to create isolated pairs of topological monopoles with the opposite topological charge and we have observed their annihilation process. When the fibre was set perpendicular to the nematic director, the monopoles were point defects in a form of radial and hyperbolic hedgehog and they attracted at small separations with an elastic force, which is proportional to the inverse square of the separation, following the Coulomb law for electric monopoles. The work was published in M. Nikkhou et al., Phys. Rev. E 93, 062703 (2016). In the case of a parallel fibre to nematic director the monopoles are in the form of Saturn ring and Saturn anti-ring. Here in thick cells we again observe a Coulomb-like attraction, while in thin cells there is an additional string-like force attributed to the formation of defect lines, connecting both monopoles. This force is independent of the separation between monopoles and prevails Coulomb-like attraction at large separations. These findings were published in M. Nikkhou et al., Phys. Rev. E 93, 062703 (2016).

We found that the dynamics of topological monopole annihilation on a fibre is very different for thick and thin nematic layers in thick cells, the two defects show a Coulomb-like pair attraction with no background force, which decays as an inverse square of the defect separation. However, for cell thickness comparable to the glass fibre diameter, there is another dominant type of force which is string-like and independent of the defect separation. It turns out that this constant force of attraction in thin cells is due to the interconnection of topological defects by additional defect lines which are running along the fibre surface. This work was published in M. Nikkhou et al., Eur. Phys. J. E 39: 100 (2016).

### Topological defects in thin nematic shells

We studied numerically topological defects (TDs) in effectively two-dimensional closed soft films exhibiting in-plane orientational ordering. We introduced the Effective Topological Charge Cancellation mechanism controlling the localized positional assembling tendency of TDs and the formation of pairs defect-antidefect on curved surfaces and/or the presence of relevant "impurities" (e.g., nanoparticles). For this purpose an effective topological charge  $m_{eff}$  is defined consisting of real, virtual and smeared curvature topological charges within a surface patch identified by the characteristic spatially averaged local Gaussian curvature  $K$ . We demonstrate a strong tendency enforcing  $m_{eff} \rightarrow 0$  on surfaces composed of surface patches exhibiting significantly different values of  $K$ . For non-zero  $m_{eff}$  we estimate a critical depinning threshold to form pairs of defect-antidefect using the electrostatic analogy. The work was presented in two invited lectures and in the publication L. Mesarec et al., Scientific Reports 6, no. 27117, 1-9 (2016).

### Biodegradable optical waveguides for use in photomedicine

A new class of optical waveguides for use in deep-tissue photomedicine were demonstrated (S. Nizamoglu, et al., *Nature Communications* 7, 10374, 2016). These waveguides were made out of biocompatible and biodegradable polymer materials, which can be implanted into the body and are naturally degraded over time. The waveguides enable the use of a number of medical laser treatments and diagnostics deep into the body, which were till now only limited to the surface due to limited penetration of light into the tissues. As an example of a possible application, laser wound closure is demonstrated, which could lead to faster healing and less scarring. Biocompatible and biodegradable waveguides can also be directly applied to other light-based diagnostics, surgery and therapeutics.

### Optical super-resolution microscopy based on microlaser particles

A novel imaging technique was developed which instead of standard fluorescent molecules, uses small lasers embedded in the sample as probes [S. Cho et al., Phys. Rev. Lett. 117, 193902 (2016)]. The main characteristics of the microlasers are their very nonlinear response to the incoming pump beam intensity. The pump beam is scanned across the sample to form a 2D or 3D image. If the pump beam is set just above the laser threshold, only microlasers exactly in the center of the beam will emit laser light. This makes it possible to achieve super-resolution as well as to get confocal images with low background without the need for pinholes. Images at a resolution six times higher than that of fluorescence-based microscopes were demonstrated by using a nanowire laser. The new technique was termed *laser particle-based stimulated emission microscopy* (LASE).

### Liquid-crystal microphotonics

We continued our studies of the possible application of liquid crystals and their structures such as droplets and fibres in photonics. We numerically demonstrated wave guiding of laser beams by birefringent profiles of the escaped topological defect lines. The radially escaped nematic director profiles of a liquid crystal with negative birefringence are able to focus and guide light with radio polarisation, whereas the opposite-azimuthal polarisation passes through unaffected. Lensing by liquid-crystal structure was also demonstrated, which could be controlled by an external electric field. The light attenuation is low and these escaped defect lines have the potential for application in photonic waveguiding. We have also studied the lasing properties of chiral nematic 3D microlasers which were polymerised, as shown in Figure X3. The lasing shows two distinct mechanisms, namely the photonic band edge lasing and lasing from the whispering gallery modes. It was demonstrated that the polarisation of the liquid crystal greatly increases the lasing stability.

We also published an extended review paper on liquid-crystal microphotonics (I. Mušević, Liquid Crystal Reviews 4, 1 (2016)). This work summarises the main aspects of liquid-crystal microphotonics including nematic colloids and liquid-crystal dispersions.

### Molecular motors

In collaboration with researchers from Dresden and Warsaw we investigated the working mechanism of the motor protein kinesin-14. Even though the main task of most cytoskeletal motors is longitudinal motion, many of them also exert a torque on their filaments, leading to helical motion. The significance of this torque is still unknown, but it might be involved in the establishment of body chirality in certain organisms. In our motility assay the motors are attached to the surface and move microtubules, whose longitudinal and angular motion is simultaneously observed through attached quantum dots and FLIC microscopy. Unexpectedly, the period of the helical motion strongly depends on the ATP concentration. We developed a minimal mechanochemical model for kinesin-14, which allows us to explain this dependence and also to reconstruct the motor's working cycle. Our results demonstrate how measurements on large ensembles can be used to infer the properties of individual molecules. The work was published in *Proc. Natl. Acad. Sci. USA* 113, E6582–E6589 (2016).

### Low-friction nanomaterials

Hard coatings have been used as wear-protection coatings for decades but without optimization of conventional lubrication systems. In the paper "Tribological performance of TiN, TiAlN and CrN hard coatings lubricated by MoS<sub>2</sub> nanotubes in Polyalphaolefin oil". Wear, vol. 352-353, p. 72, by S. Paskvale, M. Remskar, M. Čekada, we reported that the addition of MoS<sub>2</sub> nanotubes in polyalphaolefin (PAO) oils leads to a significant reduction in friction and to a decrease in the wear behaviour of tool steel AISI D2 coated with TiN, TiAlN and CrN hard coatings. Comparative tests using conventional MoS<sub>2</sub> platelets in PAO oil was performed on these hard coatings. In all cases, the MoS<sub>2</sub> nanotubes substantially decreased friction (on CrN for 55%, on TiN for 65%, and on TiAlN for 25%), while the MoS<sub>2</sub> platelets were less efficient or even increased friction.

In the paper *Transitioning to sustainable production - Part III: developments and possibilities for integration of nanotechnology into material processing technologies* (P. Krajnik et al., J. of Cleaner Production 112, 1156 (2016)) we reported on the superior tribological properties of cooling-lubricating fluids based on biodegradable vegetable oils with added functionalized MoS<sub>2</sub> nanotubes, to those of conventional metalworking fluids.

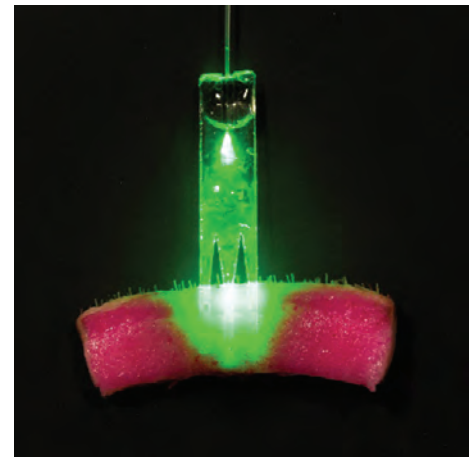


Figure 22: A biodegradable optical waveguide through which green laser light is sent into a piece of skin tissue.

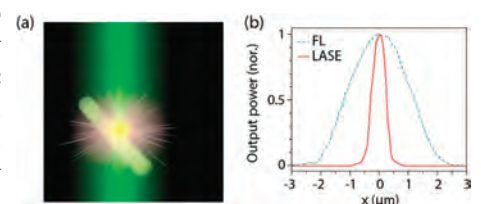


Figure 23: (a) Artistic view of a nanowire microlaser illuminated by an external beam of light. (b) Comparison of resolution between regular fluorescence imaging and the new LASE microscopy.

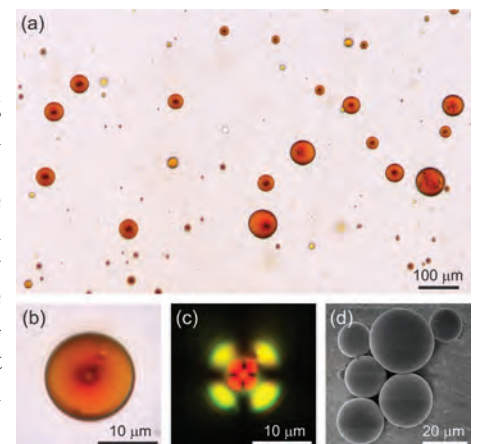


Figure 24: Dispersion of polymerised chiral nematic droplets in glycerol. They are red because the DCM fluorescent dye was added to a liquid crystal. The lower panels show examples of droplets and SEM image of a cluster of polymerised and dried microlasers.

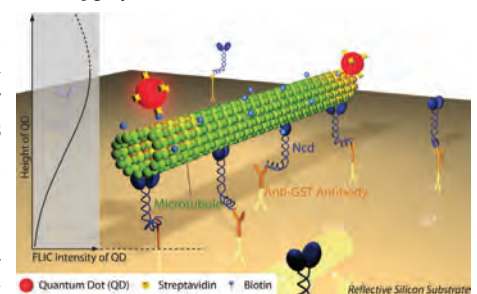


Figure 25: Measurement of longitudinal and rotational motion of microtubules using quantum dots and FLIC microscopy.

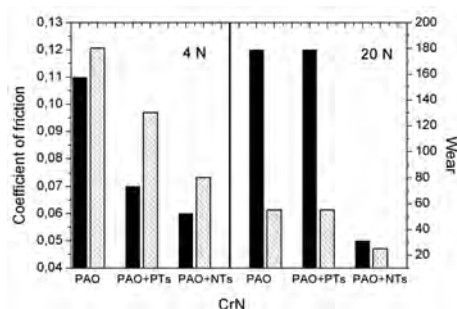


Figure 26: Coefficients of friction and wear at the 4N and 20N loads at the contact between CrN hard coating and steel (100Cr6) ball. We used the following lubricants: pure PAO oil, PAO oil with 2 wt. % of MoS<sub>2</sub> nanotubes (PAO+NTs) or standard MoS<sub>2</sub> platelets (MoS<sub>2</sub>+PTs).



Figure 27: STM picture of a superstructure in graphene lying on graphite substrate.

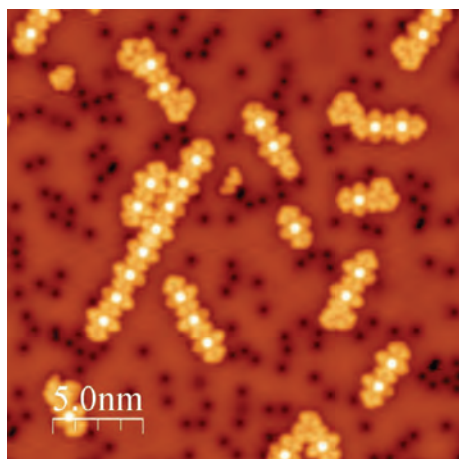


Figure 28: High-resolution STM image showing molecular chains of organic BETS and GaCl<sub>4</sub> molecules on Ag(111) surface (25 × 25 nm<sup>2</sup>, T=4.2K)

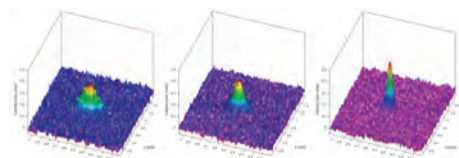


Figure 29: Velocity-distribution images showing about 50,000 caesium atoms being evaporative cooled to temperatures around 1 nK, where the transition to a Bose-Einstein condensate occurs.

### Low-dimensional materials

Molybdenum trioxide, MoO<sub>3</sub>, belongs to semiconductors with a wide energy band gap. It is used in photovoltaics, as sensors and for energy storage. In the article "Oxygen deficiency in MoO<sub>3</sub> polycrystalline nanowires and nanotubes", Materials Chemistry and Physics 170 (2016) 154, by A. Varlec, D. Arčon, S.D. Škapin and M. Remškar, we reported on the first synthesis route of the orthorhombic MoO<sub>3</sub> nanotubes by oxidation of molybdenum-sulphur-iodine nanowires. Oxygen deficiency was determined by electron-paramagnetic resonance observing paramagnetic defects (Mo<sub>5+</sub>) and explained using Raman spectroscopy by appearance of a new resonant band (1004 cm<sup>-1</sup>).

Superstructures observed by scanning tunnelling microscopy on graphite have been reported several decades ago, but the interest in these superstructures recently intensified due to their occurrence in graphene grown on different substrates. In the article *Influence of surface defects on superlattice patterns in graphene on graphite* (M. Remškar and J. Jelenc, Surface Science 651, 51 (2016)) we reported experimental findings that the orientation of the superstructure is influenced by surface defects and edges of graphene. Superstructures in graphene put on graphite exist even if the graphene is not supported by graphite over its entire area. The modulation of the density of states influences the strength of intra-layer carbon bonds in such a way that the graphene breaks along the superstructure minima.

### Nanosafety

In the telecast *When science explodes*, aired on the national television (Slo1) on 17 Dec, 2016 as a part of education program *Bite into science*, and in the telecast *Black market flourishes, fireworks also have a dark side* aired by a commercial TV (POP TV) in broadcast *Inspector* on Dec. 22, 2016, M. Remškar reported on air pollution by nanoparticles released during use of fireworks and sparklers.

### Small structures and 1D chains of organic molecules

By carefully controlling the growth conditions, we can fabricate different nanostructures and 1D chains of organic BETS molecules (Fig. ) on silver (111) surfaces. We are studying the structure and properties of such formations using low-temperature scanning tunnelling microscopy and spectroscopy. We measured a narrow gap in the density of states, which indicates the chains to be semiconducting. As previously observed on monolayer islands, grown from same material (single crystals of (BETS)<sub>2</sub>GaCl<sub>4</sub>), the GaCl<sub>4</sub> molecules can fill the gaps between pairs of BETS molecules and greatly influence the electronic properties of molecular chains.

### Ultra-cold atoms

For the first time in the Laboratory for Cold Atoms at Jožef Stefan Institute caesium atoms were evaporative cooled to temperatures of about 1 nK. Simultaneously, their density was increased, which leads to formation of Bose-Einstein condensate (Figure 29). Currently, we are trying to increase the number of atoms in the condensate and to achieve the condensation at even higher temperatures.

## III. Research program "Experimental biophysics of complex systems and imaging in biomedicine"

The program "Experimental biophysics of complex systems and imaging in biomedicine" combines the research of the processes and structure of the biological systems with the development of advanced experimental techniques, especially microspectroscopies, super-resolution microscopies, and imaging techniques. Our group is mainly focused on understanding the response of the molecular and supra-molecular structures to the interaction between materials and living cells, and to the interaction between light and living cells. We are interested in mechanisms of this response, time scales and conditions as well as its application in medicine, especially in the field of medical materials and devices, and in healthcare in general. With the development of spectroscopic, microscopic and microspectroscopic techniques, we aim to provide a new understanding of biological systems, which will open up new possibilities in the design of novel medical devices for therapy, diagnostics and regeneration – one of the main health issues among the aging population of the developed world. Our group mastered various spectroscopic techniques, such as the EPR and FTIR, microscopic and microspectroscopic fluorescence techniques such as FMS and many special MRI techniques and we have introduced super-resolution microscopic techniques such as the STED, FCS and STED

FCS, together with the novel two-photon STED and spectral sensitive STED. Among the methods of magnetic resonance imaging, a new method, which enables the monitoring of the electric field in tumours during their treatment by electroporation high-voltage electric pulses, has been developed. In addition, we have developed a method of multiparametric magnetic resonance imaging, which has been found to be very efficient in the characterization of food, drugs and various processes. By using high spatial resolution magnetic resonance imaging, we can monitor the efficiency of the surface treatment, formation and dissolution of gel layers as well as diffusion measurements in samples with restricted geometry.

#### Cell-material interaction studies

The cell-material interaction studies, especially from the viewpoint of bioactivity and biocompatibility, are undoubtedly one of the hottest biophysics research topics. We have previously shown that titanium dioxide nanoparticles strongly interact with lipid membranes from either model vesicles or even live cells – they can adsorb to the membrane and wrap themselves by a lipid corona. We have recently indisputably corroborated this idea with additional experiments using original approaches, such as fluorescence (micro)spectroscopy with in-house-designed and synthesized environment sensitive molecular probes, and state-of-the-art biophysical methods, such as fluorescence cross-correlation spectroscopy (FCCS) and super-resolution fluorescence imaging (STED). For the latter two, we teamed with the renowned prof. Christian Eggeling from the University of Oxford (UK) to foster the transfer of knowledge on these advanced techniques, which will also be available in our laboratory.

Many studies on the safety of engineered nanomaterials focused only on finding correlations between nanomaterial properties and adverse health outcomes, without taking into account underlying molecular events. A consortium of research institutions (including our group) and companies teamed up for the SmartNanoTox project with a common goal of identifying molecular initiating events and key events on a cellular level and connecting them to adverse health outcomes after inhalation of the nanomaterial. This approach should therefore yield a mechanistic picture of nanomaterial toxicity, which will lead to the discovery of causal links between molecular initiating events from the *in-vitro* models and the adverse health outcomes determined with animal models. Using the existing literature, we have identified the most suitable cell-based and cell-free *in-vitro* models of the lung. Some of the molecular initiating events identified are: nanomaterial – lipid interaction including corona formation after exposure of a nanoparticle to lung surfactant, cellular uptake of nanoparticles, and lysosomal destabilization. We have successfully labelled  $\text{TiO}_2$  nanotubes with different fluorophores, which are also suitable for high-resolution STED imaging. Our preliminary data show that the nanotubes enter the cells as single nanotubes – an event that cannot be resolved from confocal microscopy (see Figure 30).

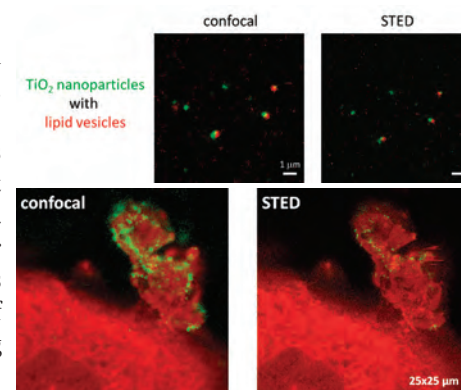
#### Fluorescence microspectroscopy (FMS)

Fluorescence microspectroscopy (FMS) reveals physical properties of molecular environment of fluorescent probes. For example, we have developed probes that are sensitive to the local pH value. They only activate at low pH. In addition, their spectral properties change, if they aggregate. There are a number of mechanisms being exploited with these probes to study molecular vicinity. Widely used is fluorescence resonance energy transfer (FRET). Lately, contact- or aggregation-based mechanisms are also being utilized. In the case of rhodamine probes, aggregate formation leads to non-fluorescent ground-state complexes or spectral shifts. With calibration of concentration and pH dependence, the developed probes will be useful for a quantitative determination of the level of aggregation, i.e., as sensors for the detection of molecular contact.

#### Multiparametric detection of the impact of the high-intensity light source on biological systems

A new experimental system for multiparametric detection of the impact of the high intensity light source on biological systems was developed. Common fluorescence detection of individual structures of the retina before and after the injury with a strongly focused high-intensity light source was changed and improved with fluorescence micro-spectral detection. The system was developed on an existing fluorescence microspectroscopy (FMS) machine with a newly installed near-IR laser source with a well-defined spatiotemporal resolution. Using this system, we were able to successfully characterize the interaction of the light source with biological matter. In addition, a new method for the localization and dynamics monitoring of blood clotting following the blood vessel injury was introduced, based on the optical tweezers and their mechanical manipulation of individual or multiple erythrocytes.

**FMS detection of the lipid wraps around the metal-oxide nanotubes has been confirmed for the first time using STED microscopy, which directly identified the entry of the particles into the cells. FMS has been used to detect the edges of a new blood clot after the laser-induced blood photocoagulation. New methods were developed to monitor food processing and food-quality control based on the multiparametric MR imaging.**



*Figure 30: Co-localization of the lipid wraps (red) and nanotubes with STED microscopy (top) of the fluorescently labelled  $\text{TiO}_2$  nanotubes (green). High resolution STED microscopy of fluorescently labelled  $\text{TiO}_2$  nanotubes (green) and a cell (red) enables direct imaging of nanoparticles entering the cell.*



To mimic the *in vivo* coagulation processes during vessel disruption, we used retinal tissue samples from *ex vivo* porcine eyes. The detection of blood coagulation was performed by the fluorescence microspectroscopy (FMS) system developed in our laboratory. In order to identify the extent of the clot formation after the accurately localized vessel rupture in the intact retina, we measured the auto-fluorescence contrast inside the blood vessel indicating a blood flow. A significant decrease in the negative contrast as detected after one minute is the result of the decreased number of erythrocytes in the volume. The observed blood flow showed the inability of the formed clot to completely seal/close the vessel. Using the negative contrast fluorescence technique, it is difficult to distinguish between the non-coagulated and coagulated region inside the ruptured vessel, but with the FMS blood-clot characterization technique, the differences between the non-coagulated blood (blue colour) and coagulated blood (green colour) in the initial clot localization could be easily observed. The measured red spectral shift of  $\Delta\lambda = 1-2$  nm in the damaged region directly indicates the changed absorption properties of hemoglobin and thus the local physio-chemical changes, which means the onset of the clot formation. We can see that part of the targeted region just below the ruptured vessel wall remains non-coagulated (blue colour).

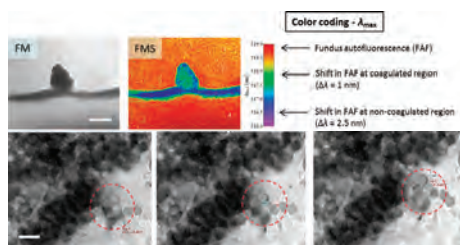


Figure 31: FMS approach to localize a blood clot 5 minutes after laser induced vessel rupture (top, scale bar is 200  $\mu\text{m}$ ) and blood clot boundary identification by optical tweezers mechanical manipulation of individual erythrocytes (bottom, scale bar is 10  $\mu\text{m}$ ). The concurrent movement of closely packed erythrocytes induced by a laser tweezers (see cross locator) is denoted within the red circle.

In order to confirm the initial clot formation, we used optical tweezers. Strong binding between individual erythrocytes a few tens of  $\mu\text{m}$  outside of the ruptured vessel formed on a minute timescale after a vessel injury. Optical tweezers manipulation in a vertical direction (See cross-locator in Figure 31), with trapping force of  $F \approx 10$  pN ( $P = 50$  mW), used the concurrent movement of a group of more than 10 closely packed erythrocytes. The optical force was unable to detach single erythrocytes from the bulk, which indicates strong adhesion, i.e., the initial state of the clot formation. For comparison, erythrocytes inside the vessel, a few tens of microns away from the ruptured site, did not aggregate. Our results show that the initial clot formation is in agreement with our hypothesis that the initial clot formation is localized to the site where the

plasma calcium concentration is decreased in the region where blood plasma is diluted with released cytoplasm of injured tissue surrounding the blood vessel.

Based on our collaboration with the Smithies' lab from the University of North Carolina and our work published in the Langmuir journal, we were invited to describe and film all the details of our method for the Size Controlled Synthesis of Stable Oligomeric Clusters of Gold Nanoparticles under Ambient Conditions (J. Vis. Exp. 2016 (108):e53388). In this work, we described how reducing dilute aqueous  $\text{HAuCl}_4$  with sodium thiocyanate ( $\text{NaSCN}$ ) under alkaline conditions produces 2–3-nm-diameter nanoparticles and stable grape-like oligomeric clusters of yellow nanoparticles. The produced yellow oligoclusters range in size from  $\sim 3$  to  $\sim 25$  nm. This size range can be further extended by an add-on method utilizing hydroxylated gold chloride ( $\text{Na}^+[\text{Au}(\text{OH}_{4-x})\text{Cl}_x]^-$ ) to autocatalytically increase the number of subunits in the as-synthesized oligocluster nanoparticles, providing a total range of 3 nm to 70 nm. We were able to concentrate the oligoclusters more than 300 fold without aggregation and the crude reaction mixtures remained stable for months without further processing.

#### Diffusion measurement by modulated gradient

We improved our method for diffusion measurement by modulated gradients. In some of our experiments, especially those on bulk liquids, we found that the method gives overestimated results for the diffusion constant with higher frequencies of modulated gradients. In the study, we showed that the origin of the error is in neglecting the off-resonance contributions to the signal of multiple spin echoes in a high magnetic field gradient. Because of these contributions, the total signal was decaying faster than was predicted by our theory, which led to the overestimated calculated diffusion constant. We found a solution to the problem in zero frequency filtering of the spin echo signals, which removed most of the off-resonance signals and therefore made our theoretical model valid again. The results of the study were published in the Journal of Magnetic Resonance, 2016, 270: 77-86.

#### Dry-curing of different meat products

By using multiparametric magnetic resonance imaging, we studied dry-curing of different meat products. Relaxation time  $T_1$  and  $T_2$  mapping, and the apparent diffusion constant (ADC) mapping were used to find the differences between two different ham muscles (biceps femoris and semimembranosus) at two different stages of salting (low and high). We showed that the maps can be converted into one-dimensional distributions of the parameters  $T_1$ ,  $T_2$  and ADC, and in two-dimensional correlations between the parameters ADC- $T_2$ , ADC- $T_1$ ,  $T_1$ - $T_2$ , which show characteristic peaks in the distribution. The location and distribution of these peaks are very sensitive to both the tissue type and the influence of the salting. The characterization was better with the two-dimensional correlation than with one-dimensional distributions. To these three mapping methods, we also added quantitative magnetization transfer imaging, which was found to be efficient for determining the protein content. We concluded that these methods, having greater accessibility to NMR / MRI systems, could serve as an effective tool for monitor-

ing the processing of dry-cured meat products, as well as to control their quality. This research, which was published in the journal *Meat Science*, 2016, 122: 109, was achieved in cooperation with the researchers from the Agricultural Institute of Slovenia. We also studied the effects of the electroporation on the properties of a potato tuber. We found that with the electric field of more than 400 V/cm, cells start to release substances, which result in an increase of T2 relaxation time. The effect was found to be larger with a higher electric field and was also larger immediately after the electroporation than several hours after it. We found no significant changes associated with electroporation in maps of the apparent diffusion constant or on the maps of T1 relaxation time. During the delivery of the electroporation pulses, we were able to monitor the electric field in the sample using the MREIT method. This enabled us to find relations between the electric field in the sample and its effect on the change of NMR relaxation parameters as well as on the diffusion constant. The findings of this study were published in the *Innovative Food Science and Emerging Technologies*, 2016, 37: 384.

#### Influence of the highly soluble pentoxifylline drug on the dynamics of medium penetration into the tablet and the formation of the gel layer in xanthan tablets

We also investigated the influence of the highly soluble pentoxifylline drug on the dynamics of medium penetration into the tablet and the formation of the gel layer in xanthan tablets.

Xanthan is an anionic polymer that exhibits pH- and ionic-strength-dependent swelling. For this reason, the impact of the medium properties on xanthan swelling has also been studied. For hydrophilic polymers, it is generally accepted that, once in contact with a body fluids, they hydrate and swell, forming a gel layer that regulates the penetration of body fluids into the tablet and the dissolution of the incorporated drug. Therefore, the knowledge of the gel layer characteristics is of crucial importance for the use of controlled drug-delivery systems. A combination of different MRI methods enables an accurate determination of the medium penetration into the tablet, as well as hydrogel formation *in situ*. The results of xanthan swelling and pentoxifylline release kinetics were compared to the mathematical model, which combines the polymer swelling kinetics and drug diffusion and solubility to obtain the release mechanism. In water and diluted acid medium (pH >3) with low ionic strength, the main release mechanism is erosion, whereas in acid medium (pH 1.2) and in media with high ionic strength ( $\mu \geq 0.2$ ), the diffusion mechanism dominates, owing to the changes in the polymer structure in media with different pH and ionic strength. The results were published in a paper entitled *The Influence of other high loading and xanthan tablets and media with Different physiological pH and ionic strength on swelling and release* in the *Journal of Molecular Pharmaceutics*, 2016, 13: 1147. This study was performed in collaboration with our colleagues from the Faculty of Pharmacy, University of Ljubljana.

#### Penetration of tung oil into various wood species

Furthermore, we studied the penetration of tung oil into various wood species. Tung oil is used as environmentally friendly wood preservatives. However, tung oil does not penetrate deeply into the wood due to its high viscosity. Magnetic resonance imaging was applied to elucidate the influence of the applied impregnation method (immersion in oil or vacuum impregnation with oil) and on the wood species used. It has been shown that the oil penetrated deeply in the wood after the impregnation process than after the immersion process, where the oil remained only on the sample surface. In addition, the depth of penetration of the oil into the wood also depends on the wood species and on the orientation of the sample. Since wood is an anisotropic material, the penetration of the oil is the largest in the axial direction. The results of the research were combined in an article accepted for publication in the *Journal Industrial Crops and Products*, 2017, 96: 149. The study was performed in collaboration with our colleagues from the Department of Biotechnical Faculty.

Our research has been supported by a number of international projects financed by the European Union. It was also supported within the bilateral Slovenian – USA, Slovenian – German and Slovenian – Greek and other scientific cooperations. In 2016, the Department had cooperation 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, Athens, Greece
- Institut für Biophysik und Nanosystemforschung OAW, Graz, Austria

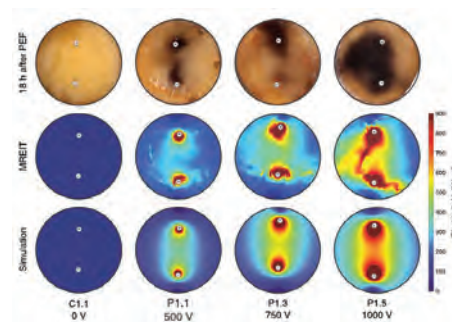


Figure 32: Electric field in the potato tuber sample established during electroporation as measured by the MREIT technique (middle row) is in a good agreement with the results of simulation (bottom row) as well as with the release of phenolic compounds that darkened due to an oxidation reaction (optical photographs in the top row). In the study voltages of electroporation pulses were 500, 750 and 1000 V.

- 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
  - 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 2016

1. A. Rešetič, J. Milavec, B. Zupančič, V. Domenici, B. Zalar. Polymer-dispersed liquid crystal elastomers. *Nature Communications* 7, 13140 (2016).
2. M. Jeong, M. Klanjšek et al. Dichotomy between attractive and repulsive tomonaga-luttinger liquids in spin ladders. *Physical Review Letters* 117, 106402 (2016).
3. F. E. Annanouch, P. Umek et al. Aerosol-assisted CVD-grown PdO nanoparticle-decorated tungsten oxide nanoneedles extremely sensitive and selective to hydrogen. *ACS Applied Materials & Interfaces* 8, 10413 (2016).
4. H. Uršič, V. Bobnar, B. Malič, C. Filipič, M. Vrabelj, S. Drnovšek, Jo Younghun, M. Wencka, Z. Kutnjak. A multicaloric material as a link between electrocaloric and magnetocaloric refrigeration. *Scientific Reports* 6, 26629 (2016).
5. M. Igarashi, P. Jeglič, A. Kranjc, R. Žitko, T. Nakano, Y. Nozue, and D. Arčon. Metal-to-insulator crossover in alkali doped zeolite. *Scientific Reports* 6, 18682 (2016).
6. G. Posnjak, S. Čopar and I. Mušević. Points, skyrmions and torons in chiral nematic droplets. *Scientific Reports* 6, 26361 (2016).
7. L. E. Aguirre, A. de Oliveira, D. Seč, S. Čopar, P. L. Almeida, M. Ravnik, M. H. Godinho, S. Žumer. Sensing surface morphology of biofibers by decorating spider silk and cellulosic filaments with nematic microdroplets. *Proc. Natl. Acad. Sci. USA* 113, 1174 (2016).
8. S. Nizamoglu, M. Humar et al. Bioabsorbable polymer optical waveguides for deep-tissue photomedicine. *Nature Communications* 7, 10374 (2016).
9. S. Cho, M. Humar, N. Martino, S. H. Yun. Laser Particle Stimulated Emission Microscopy. *Phys. Rev. Lett.* 117, 193902 (2016).
10. B. Nitzsche, E. Dudek, L. Hajdo, A. A. Kasprzak, A. Vilfan, S. Diez. Working stroke of the kinesin-14, ncd, comprises two substeps of different direction. *Proc. Natl. Acad. Sci. USA* 113, E6582 (2016).

### Some outstanding publications in 2015

1. M. Sluban, P. Umek, Z. Jagličič, J. Buh, P. Šmitek, C. Bittencourt, P. Guttman, M.-H. Delville, D. Mihailović, D. Arčon. Controlling disorder and superconductivity in titanium oxynitride nanoribbons with anion exchange. *ACS Nano* 9 (2015), 10133.
2. M. Pregelj, A. Zorko, O. Zaharko, H. Nojiri, H. Berger, L. Chapon, D. Arčon. Spin-stripe phase in a frustrated zigzag spin-1/2 chain. *Nature Communications* 6, 7255(2015).
3. M. Klanjšek, D. Arčon, A. Sans, P. Adler, M. Jansen, C. Felser. Phonon-modulated magnetic interactions and spin Tomonaga-Luttinger liquid in the p-orbital antiferromagnet CsO<sub>2</sub>. *Physical Review Letters* 115, 057205(2015).
4. R. H. Zadik, A. Potočnik, P. Jeglič, D. Arčon, et al. Optimized unconventional superconductivity in a molecular Jahn-Teller metal. *Science Advances* 1, e1500059(2015).
5. M. Pregelj, A. Zorko, M. Gomilšek, et al. Controllable broadband absorption in the mixed phase of metamagnets. *Advanced Functional Materials* 25, 3634 (2015).
6. M. Nikkhou, M. Škarabot, S. Čopar, M. Ravnik, S. Žumer, I. Mušević. Light-controlled topological charge in a nematic liquid crystal. *Nature Physics* 11, 183 (2015).
7. S. Čopar, U. Tkalec, I. Mušević, S. Žumer. Knot theory realizations in nematic colloids. *Proc. Natl. Acad. Sci.* 112, 1675 (2015).

8. R. Podlipec, J. Štrancar. Cell-scaffold adhesion dynamics measured in first seconds predicts cell growth on days scale - optical tweezers study. *ACS Applied Materials & Interfaces* 7, 6782(2015).
9. T. Koklič, R. Chattopadhyay, R. Majumder, B. R. Lenz. Factor Xa dimerization competes with prothrombinase complex formation on platelet-like membrane surfaces. *Biochemical Journal* 467, 37(2015).
10. Z. Arsov, U. Švajger, J. Mravljak, S. Pajk, A. Kotar, I. Urbančič, J. Štrancar, M. Anderluh. Internalization and accumulation in dendritic cells of a small pH-activatable glycomimetic fluorescent probe as revealed by spectral detection. *ChemBioChem* 16, 2660(2015).

### Some outstanding publications in 2014

1. A. Zorko, O. Adamopoulos, M. Komelj, D. Arčon, A. Lappas. Frustration-induced nanometre-scale inhomogeneity in a triangular antiferromagnet. *Nature Comms* 5, 3222 (2014).
2. P. Koželj, S. Vrtnik, A. Jelen, S. Jazbec, Z. Jagličič, S. Maiti, M. Feuerbacher, W. Steurer, J. Dolinšek, *Phys. Rev. Lett.* 113, 107001 (2014).
3. R. Pirc, B. Rožič, J. Koruza, B. Malič, Z. Kutnjak, Negative electrocaloric effect in antiferroelectric PbZrO<sub>3</sub>. *Europhysics Letters* 107, 17002-1-5(2014).
4. A. Martinez, M. Ravnik, B. Lucero, R. Visvanathan, S. Žumer, and I.I. Smalyukh Mutually tangled colloidal knots and induced defect loops in nematic fields, *Nature Mater.* 13, 258-263 (2014).
5. D. Seč, S. Čopar and S. Žumer, Topological zoo of free-standing knots in confined chiral nematic fluids, *Nature Comms.* 5, 3057 (2014).
6. J. Dontabhaktuni, M. Ravnik and S. Žumer, Quasicrystalline tilings with nematic colloidal platelets, *Proceedings of the National Academy of Sciences of the United States of America* 111, 2464 (2014).
7. S. Čopar, Topology and geometry of nematic braids, *Phys. Rep.* 538, 1-37 (2014).
8. A. Vilfan, 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).

### Awards and appointments

1. Dr. Matjaž Humar: 1st Place Poster Prize at prestigious Nobel Laureate Meeting 2016, Lindau, Germany. Matjaž presented a poster about lasers embedded into single live cells for the first time. He has also demonstrated that fat cells already present in the human body already contain tiny lasers, which only need to be activated.
2. Dr. Matjaž Humar: Bronze Award from community Šempeter-Vrtojba for 2016, Šempeter-Vrtojba. The prize for the high successes in the world scale in recent years and as a stimulation for further scientific work.
3. dr. Janez Pirš, Honorary distinction of "Jožef Stefan" Institute, Ljubljana, Slovenia, Honorary distinction for his successful contribution for developing new high-tech products based on scientific and technological achievements of the 'Jožef Stefan' Institute.

### Organization of conferences, congresses and meetings

1. 6th Workshop on Liquid Crystals for Photonics, 14. 9. - 16. 9. 2016, Ljubljana, Slovenia
2. 10. Conference of physicists in basic research, 16. 11. 2016, Otočec, Slovenia

### Patent granted

1. Igor Muševič, Matjaž Humar, Spherical liquid-crystal laser, US9263843 (B2), US Patent Office, 16. 02. 2016

## INTERNATIONAL PROJECTS

- 7FP - ESNSTM; Electron Spin Noise Scanning Tunneling Microscopy  
Prof. Janez Dolinšek  
European Commission
- 7FP - NanoMag; Magnetic Nanoparticles and Thin Films for Spintronic Applications and High Performance Permanent Magnets  
Prof. Janez Dolinšek  
European Commission
- 7FP - SIMDALEE2; Sources, Interaction with Matter Detection and Analysis of Low Energy Electrons 2  
Prof. Maja Remškar  
European Commission
- 7FP - LIVINGLASER; A Laser made Entirely of Living Cells and Materials derived from Living Organisms  
Prof. Igor Muševič  
European Commission
- 7 FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability  
Prof. Maja Remškar  
European Commission
- COST MP1201; Rational Design of Hybrid Organic-Inorganic Interfaces: The Next Step Towards Advanced Functional Materials  
Dr. Polona Umek  
Cost Office
- COST CA15107; Multi-Functional Nano-Carbon Composite Materials Network  
Dr. Polona Umek  
Cost Office
- COST CA15209; European Network on NMR Relaxometry  
Prof. Tomaž Apih  
Cost Office
- COST CA16109; Chemical On-Line cOmpoSiton and Source Apportionment of fine aerosol  
Dr. Griša Močnik  
Cost Office
- H2020 - SmartNanoTox; Smart Tools for Gauging Nano Hazards  
Prof. Janez Štrancar  
European Commission
- Solar Cell Application of Rf Rotating Plasma Modified Inorganic Nanotubes  
Prof. Maja Remškar  
Slovenian Research Agency
- Spin-liquid Ground State of Quantum Kagome Antiferromagnets from a Local-probe Perspective  
Asst. Prof. Andrej Zorko  
Slovenian Research Agency
- Controlled Nanoparticle Assemblies in Complex Soft Matrices  
Prof. Samo Kralj  
Slovenian Research Agency
- Investigating Catalytic and Physical Properties of CuGdCa Alloys  
Prof. Tomaž Apih  
Slovenian Research Agency
- Aromatic Polymers with Ultrahigh Breakdown Field Strength, Low Dielectric Loss, and High Electric Energy Density  
Prof. Zdravko Kutnjak  
Slovenian Research Agency
- Investigation of Complex Materials for Hydrogen Storage  
Prof. Janez Dolinšek  
Slovenian Research Agency
- Lipid Wrapped Gold Nanoparticles and Activity of Factor Xa  
Prof. Janez Štrancar  
Slovenian Research Agency
- Crystal and Electronic Structure of NbS<sub>3</sub> Phases  
Dr. Erik Zupanič  
Slovenian Research Agency
- Radiative forcing of desert mineral dust and PM10 concentrations over Southern Europe  
Prof. Maja Remškar  
Slovenian Research Agency
- Lead-free (Ba<sub>0.8</sub>Ca<sub>0.2</sub>)<sub>1-x</sub>La<sub>2x</sub>/3TiO<sub>3</sub> based electrocaloric materials for new dielectric cooling technologies  
Prof. Zdravko Kutnjak  
Slovenian Research Agency
- Stabilisation of lattices of topological defects  
Prof. Samo Kralj  
Slovenian Research Agency

## RESEARCH PROGRAMS

- Physics of Soft Matter, Surfaces and Nanostructures  
Prof. Slobodan Zumer
- Experimental Biophysics of Complex Systems  
Prof. Janez Štrancar
- Magnetic resonance and dielectric spectroscopy of „smart“ new materials  
Prof. Janez Dolinšek

## R & D GRANTS AND CONTRACTS

- Topology and Photonics of Liquid Crystal Colloids and Dispersions  
Prof. Igor Muševič
- Thermophoretic guidance, accumulation and sorting of biomolecules in microfluidic devices  
Asst. Prof. Andrej Vilfan
- Intra-pocket-targeted nanomedicines for treatment of periodontal disease  
Prof. Maja Remškar
- New advanced electrocaloric materials for novel environmentally-friendly dielectric refrigeration technology  
Prof. Zdravko Kutnjak
- The textural analysis of spatiotemporal changes for breast lesions diagnosis on ultrafast breast MRIs  
Prof. Igor Serša
- Role of Calcium and lipid membranes in survival of critically ill patients  
Dr. Tilen Koklič
- Multifunctional materials for actuator and cooling devices  
Prof. Zdravko Kutnjak
- High-Entropy Alloys  
Dr. Stanislav Vrtnik
- Metamaterials from liquid crystal colloids  
Asst. Prof. Miha Ravnik
- Optimization strategies in biological and artificial microfluidic systems  
Asst. Prof. Andrej Vilfan
- Selective and hypersensitive microcapacitive sensor system for targeted molecular detection in the atmosphere  
Prof. Igor Muševič
- Correlated electrons in confined molecular systems  
Prof. Denis Arčon
- Water exclusion efficacy, measure for prediction of wood performance against wood decay fungi  
Prof. Igor Serša
- Micro-electromechanical and electrocaloric layer elements  
Prof. Zdravko Kutnjak
- Performance of wood and lignocelulosic composites in outdoor applications  
Prof. Igor Serša
- Advanced electrocaloric energy conversion  
Prof. Zdravko Kutnjak
- Microspectroscopy-based optimization of the effects of laser pulses on the retina  
Prof. Janez Štrancar
- SCOPES; Spin-liquid and Spin-ice States in Frustrated Rare-earth and Transition Metal Spinels  
Dr. Matej Pregelj  
Snf-Swiss National Science Foundation
- Irradiation and Analysis of Nano SiC Samples  
Prof. Vid Bobnar  
National Nuclear Research Center
- Building blocks, tools and systems for the Factories of the Future – GOSTOP  
Prof. Janez Štrancar

## NEW CONTRACTS

- MRI scanning of samples  
Prof. Igor Serša  
KRKA, TOVARNA ZDRAVIL, D.D.
- Analyzes with nuclear quadrupole resonance (NQR)  
Prof. Tomaž Apih  
LEK d.d.
- Measurement of optical transmissivity  
Prof. Igor Muševič  
RLS Merilna tehnika d.o.o.
- Microspectroscopy-based optimization of the effects of laser pulses on the retina  
Prof. Janez Štrancar  
OPTOTEK d.o.o.

## VISITORS FROM ABROAD

- dr. Mutsuo Igarashi, Gunma National College of Technology, Maebashi, Japan, 16. 1. 2016 – 24. 1. 2016, 21. 8. 2016 – 2. 9. 2016
- mag. Kushtrim Podrimqaku, University of Pristina, Pristina, Kosovo, 21. 1. 2016 – 27. 1. 2016
- mag. Valon Veliu, University of Pristina, Pristina, Kosovo, 21. 1. 2016 – 27. 1. 2016
- dr. Uliana Ognysta, Institute of Physics, National Academy of Science of Ukraine, Kiev, Ukraine, 31. 1. 2016 – 10. 3. 2016
- dr. Vaida Lunkuviene, Faculty of Natural Sciences of Vilnius University, Vilnius, Litva, 1. 2. 2016 – 31. 3. 2016
- dr. Alicja Filipek, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland, 20. 2. 2016 – 5. 3. 2016
- dr. Alan Soper, ISIS Facility STFC Rutherford Appleton Laboratory, Harwell, Oxford, Great Britain, 1. 3. 2016 – 5. 3. 2016
- dr. Randall Kamien, University of Pennsylvania, Philadelphia, USA, 6. 3. 2016 – 9. 3. 2016
- dr. Tina Pavlin, University of Bergen, Bergen, Norway, 4. 4. 2016 – 10. 4. 2016
- dr. Surajit Dhara, School of Physics University of Hyderabad, Talangana, India, 7. 5. 2016 – 11. 6. 2016
- doc. dr. Michael Grbic, Faculty of Science, University of Zagreb, Zagreb, Croatia, 16. 5. 2016
- dr. Katarina Butalović, Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, 1. 6. 2016 – 3. 6. 2016
- dr. Milijana Savić, Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, 1. 6. 2016 – 3. 6. 2016
- dr. Manel Rodriguez Ripoll, AC2T research GmbH, Wiener Neustadt, Austria, 7. 6. 2016
- dr. Bouchra Asbani, Universite de Picardie Jules Verne, Laboratoire de la Mateiere Condense (LPMC), Amiens, France, 11. 7. 2016 – 8. 8. 2016
- dr. Mutsuo Igarashi, Gunma National College of Technology, Maebashi, Japan, 21. 8. 2016 – 2. 9. 2016, 27. 10. 2016 – 8. 11. 2016
- prof. dr. Christian Eggeling, Weatherall Institute of Molecular Medicine, Radcliffe Department of Medicine – Investigative Medicine, University of Oxford, Great Britain, 24. 8. 2016 – 27. 8. 2016
- dr. Carla Bittencourt, University of Mons, Mons, Belgium, 7. 9. 2016 – 31. 10. 2016
- dr. Jun-ichi Fukuda, Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, 11. 9. 2016 – 6. 10. 2016
- dr. Sergey Lushnikov, AF Ioffe Physicotechnical Institute, RAS, St. Petersburg, Russia, 3. 10. 2016 – 31. 10. 2016
- dr. Magdalena Wencka, Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland, 19. 10. 2016 – 28. 10. 2016
- prof. dr. Francesco Sagues, University of Barcelona, Barcelona, Spain, 26. 10. 2016 – 28. 10. 2016
- prof. Eung Je Woo, Kyung Hee University, Seoul, Korea, 13. 11. 2016 – 19. 11. 2016
- dr. Ana Varlec, APE Research, Area Science Park, Basovizza, Italy, 20. 11. 2016 – 2. 12. 2016

## STAFF

### Researchers

- Prof. Tomaž Apih
- Prof. Denis Arčon\*
- Asst. Prof. Zoran Arsov
- Prof. Vid Bobnar
- Prof. Janez Dolinšek\*
- Dr. Cene Filipič
- Dr. Anton Gradišek
- Dr. Alan Gregorovič
- Abdelrahim Ibrahim Hassanien, B. Sc.
- Dr. Peter Jeglič
- Dr. Martin Klanjšek
- Dr. Tilen Koklič
- Dr. Georgios Kordogiannis, left 01.10.16*
- Prof. Samo Kralj\*
- Prof. Zdravko Kutnjak
- Dr. Mojca Urška Mikac
- Asst. Prof. Griša Močnik\*
- Asst. Prof. Aleš Mohorič\*
- Prof. Igor Mušević\*, Head**
- Dr. Andriy Nych
- Dr. Matej Pregelj
- Asst. Prof. Miha Ravnik\*
- Prof. Maja Remškar
- Prof. Igor Serša
- Asst. Prof. Miha Škarabot
- Prof. Janez Štrancar
- Asst. Prof. Uroš Tkalec\*
- Dr. Polona Umek
- Dr. Herman Josef Petrus Van Midden
- Asst. Prof. Andrej Vilfan
- Prof. Boštjan Zalar
- Prof. Aleksander Zidanšek
- Asst. Prof. Andrej Zorko
- Prof. Slobodan Žumer
- Postdoctoral associates**
- Dr. Franci Bajd
- Dr. Jerneja Milavec
- Dr. Giorgio Mirri\*
- Dr. Maryam Nikkhou, left 01.07.16*
- Dr. Stane Paik\*
- Dr. Rok Podlipec
- Dr. Brigita Rožič
- Dr. Anna Ryzhkova
- Dr. Iztok Urbančič
- Dr. Jernej Vidmar\*
- Dr. Stanislav Vrtnik
- Dr. Erik Zupanič

### Postgraduates

- Matjaž Gomilšek, B. Sc.
- Urška Gradišar Centa, B. Sc.
- Saša Harkai, B. Sc.
- Dr. Matjaž Humar
- Uroš Jagodič, B. Sc.
- Nejc Janša, B. Sc.
- Tilen Knaflič, B. Sc.
- Primož Koželj, B. Sc.
- Mitja Krnel, B. Sc.
- Marta Lavrič, B. Sc.
- Janez Lužnik, B. Sc.
- Bojan Marin\*, M. Sc.
- Aleksander Matavž, B. Sc.
- Tadej Mežnaršič, B. Sc.
- Maruša Mur, B. Sc.
- Luka Pirker, B. Sc.
- Gregor Posnjak, B. Sc.
- Andraž Rešetič, B. Sc.
- Muhammad Saqib, B. Sc.
- Melita Sluban, B. Sc.
- Jan Šömen, B. Sc., left 15.02.16*
- Maja Trček, B. Sc.
- Marion Antonia Van Midden, B. Sc.
- Dr. Ana Varlec, left 01.03.16*
- Technical officers**
- Dr. Luka Drinovec\*
- Dr. Maja Garvas
- Dr. Andreja Jelen
- Dr. Andraž Kocjan
- Boštjan Kokot, B. Sc.
- Ivan Kvasić, B. Sc.
- Jože Luzar, B. Sc.
- Hana Majaron, B. Sc.
- Jaka Močivnik, B. Sc.
- Technical and administrative staff**
- Dražan Ivanov
- Janez Jelenc, B. Sc.
- Maša Kavčič
- Davorin Kotnik
- Sabina Krhlikar, B. Sc.
- Silvano Mendizza
- Janja Milivojevič
- Iztok Ograjšek, retired 15.01.16*
- Ana Sepe, B. Sc.
- Marjetka Tršinar

Note:

\* part-time JSI member

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# DEPARTMENT FOR COMPLEX MATTER

F-7

*The research within the Department for Complex Matter encompasses a variety of research fields, ranging from the synthesis of new materials to fundamental investigations of elementary excitations in complex systems. These include anything from nano-biosystems to exotic 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 important discoveries 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 semiconducting transition-metal dichalcogenides and molecular nanowires, crossing into the physics and nanoscience of macromolecular biological systems venturing also into fields of quantum molecular electronics and nano-electronics. These and other materials, such as strongly correlated systems, electronically ordered systems and superconductors were investigated using advanced femtosecond spectroscopy techniques. In a number of areas we have introduced new materials, technologies and techniques.

Particular emphasis is placed on investigations of phase transitions in time, and most recently into the creation of new states of matter created under non-equilibrium conditions.

## Ultrafast studies of electron dynamics in correlated systems

In the past two decades non-equilibrium spectroscopies have evolved from avant-garde studies to crucial tools for expanding our understanding of the physics of strongly correlated materials. The possibility of obtaining simultaneously spectroscopic and temporal information has led to insights that are complementary to (and in several cases beyond) those attainable by studying the matter at equilibrium. From this perspective, multiple phase transitions and new orders arising from competing interactions are benchmark examples where the interplay among electrons, lattice and spin dynamics can be disentangled because of the different timescales that characterize the recovery of the initial ground state. For example, the nature of the broken-symmetry phases and of the bosonic excitations that mediate the electronic interactions, eventually leading to superconductivity or other exotic states, can be revealed by observing the sub-picosecond dynamics of impulsively excited states. Furthermore, recent experimental and theoretical developments have made it possible to monitor the time-evolution of both the single-particle and collective excitations under extreme conditions, such as those arising from strong and selective photo-stimulation. These developments are opening the way for new, non-equilibrium phenomena that can eventually be induced and manipulated by short laser pulses.

As the field of ultrafast spectroscopy has moved from the avant-garde to the mainstream, and has become an important tool for the study of many body and single-particle relaxation phenomena, as well as material science in general, we have completed an extensive review of the subject. The most recent achievements in the experimental and theoretical studies of the non-equilibrium electronic, optical, structural and magnetic properties of correlated materials are published in *Advances in Physics* 65, 58-238 (2016). The paper, of more than 180 pages, presents different viewpoints, from phenomenology to non-equilibrium quantum dynamics.

Systems that rapidly evolve through symmetry-breaking transitions on timescales comparable to the fluctuation timescale of single-particle excitations may behave very differently than under controlled near-ergodic conditions.

A real-time investigation with high temporal resolution can reveal new insights into the ordering through the transitions that are not available in static experiments. We investigated the system trajectory through a normal-to-superconductor transition in a prototype high-temperature superconducting cuprate in which such a situation occurs. Using a multiple pulse femtosecond spectroscopy technique we measured the system trajectory and time-evolution of the single-particle excitations through the transition in  $\text{La}_{1.9}\text{Sr}_{0.1}\text{CuO}_4$  and compared the data to a simulation based on time-dependent Ginzburg-Landau theory, using laser excitation fluence as an adjustable parameter controlling the quench conditions in both experiment and theory. The comparison revealed the presence of



Head:  
**Prof. Dragan D. Mihailović**



**European Research Council**  
Established by the European Commission

**The ultrafast non-equilibrium phenomena of superconductors have become a widely used method for the investigation of such materials. The culmination of research on ultrafast phenomena in superconductors starting in the early 1990s by our group is the publication of a 180-page review article in *Advances in Physics* and a news and views article in *Nature Materials* 15, 930-931 (2016).**

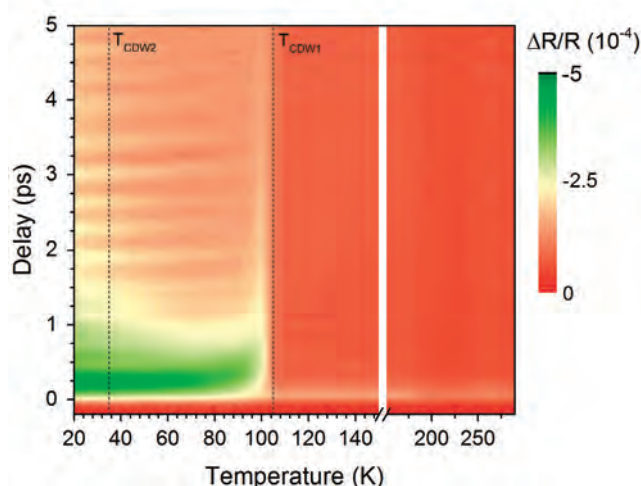


Figure 1: Temperature dependence of the transient reflectivity in  $\text{Mo}_4\text{O}_{11}$ . The vertical dashed lines indicate the CDW transition temperatures:  $T_{\text{CDW1}} = 105 \text{ K}$  and  $T_{\text{CDW2}} = 35 \text{ K}$ . The appearance of collective oscillatory modes is observed below  $T_{\text{CDW1}}$ .

charge density wave (CDW) transition at  $T_{\text{CDW1}} = 105 \text{ K}$  associated with a hidden one-dimensional Fermi surface (FS) nesting. In contrast, the appearance of the second transition at  $T_{\text{CDW2}}$  associated with further CDW ordering is barely perceptible. The coherent response can be described well by the displacive coherent excitation model of Zeiger et al. assuming a coupling of phonons to the photo-excited quasiparticles. The coupling of the collective modes to the electronic order parameter was found to be weak. The exponential relaxation was discussed in terms of single-particle relaxation and an overdamped collective mode. The manuscript has been submitted to *Phys. Rev. B* 93, 125123 (2016).

#### Ultrafast memory materials

An important new area of research is related to the search for new metastable states that have both fundamental and practical importance. The functionality of computer memory elements is currently based on multi-stability, driven either by locally manipulating the density of electrons in transistors or by switching magnetic or ferroelectric order. Another possibility is switching between metallic and insulating phases by the motion of ions, but their speed is limited by slow nucleation and inhomogeneous percolative growth. Here we demonstrate fast resistance switching in a charge density wave system caused by pulsed current injection. As a charge pulse travels through the material, it converts a commensurately ordered polaronic Mott insulating state in  $1T\text{-TaS}_2$  to a metastable electronic state with textured domain walls, accompanied by a conversion of polarons to band states, and concurrent rapid switching from an insulator to a metal. The large resistance change, high switching speed (30 ps) and ultralow energy per bit opens the way to new concepts in non-volatile memory devices manipulating all-electronic states as reported in *Nature Communications* 7, 11442 (2016). An introductory article by Mihailovic in *Nature Materials* describes a new way of tailoring phase diagrams to produce metastable phases with the help of substrate strain. The method was previously reported by Svetin et al in *Appl. Phys. Express*.

**The search for a metastable state switched by ultrafast laser pulses or electrical pulses has led to the patenting and publication in Nat. Comm. of a new type of ultrafast memory element with a world-record speed and ultra-low switching energy.**

#### Theoretical studies on the nanoscale

We develop a theory of the upper critical field in a BCS superconductor with a non-local interaction between electrons. We have shown that the non-local interaction is characterized by the universal dimensionless parameter  $k_{\text{FPD}}$ , where  $k_F$  is the Fermi momentum and  $\rho_0$  is the radius of electron-electron interaction. The presence of the external magnetic field leads to the generation of additional components of the order parameter with different angular momenta. This effect leads to the enhancement of the upper critical field above the orbital limiting field. In addition, the upward curvature in the temperature dependence of the upper critical field in the clean limit is predicted. The impurity scattering suppresses the effect in the dirty limit. (*Physical Review B* 94, 174506 (2016)).

We have developed a theoretical model in order to describe the polaron ordering on a triangular lattice. The model takes into account the short range attraction between polarons due to lattice deformation and long-range

significant superconducting fluctuations which precede the transition on short timescales. By including superconducting fluctuations as a seed for the growth of superconducting order we can obtain a satisfactory agreement of the theory with the experiment. Remarkably, the pseudogap excitations apparently play no role in this process, as described in *Phys. Rev. B* 93, 224520 (2016).

We investigated the temperature- and fluence-dependent dynamics of the time-resolved optical reflectivity in undoped spin-density-wave (SDW) and doped superconducting (SC)  $\text{EuFe}_2(\text{As,P})_2$  with an emphasis on the ordered  $\text{Eu}^{2+}$ -spin temperature region. The data indicate that in  $\text{EuFe}_2(\text{As,P})_2$  the SDW order coexists at low temperature with the SC and  $\text{Eu}^{2+}$ -ferromagnetic order. Increasing the excitation fluence leads to a slow thermal suppression of the  $\text{Eu}^{2+}$ -spin order due to the crystal-lattice heating on a nanosecond timescale, while the SDW order is suppressed non-thermally on a sub-picosecond timescale at a higher fluence, as described in *Phys. Rev. B* 94, 144519 (2016).

We conducted a systematic study of the single-particle and collective excitations by femtosecond transient reflectivity measurements in the single crystals  $\eta\text{-Mo}_4\text{O}_{11}$ , investigating the dynamics as a function of temperature with two different pump photon energies (3.1 eV and 1.55 eV). A remarkable slowing down of the relaxation dynamics was observed at the first

Coulomb repulsion. In addition to that we introduce the modulation due to charge density wave ordering. Monte Carlo simulations show that the resulting patterns are similar to that observed in the STM experiments on TaS<sub>2</sub>.

### Nanomaterials

We investigate the optical and electronic properties of transition-metal dichalcogenides (TMDs) and chalcogenides as well as oxides and carbides synthesized from them, in various low-dimensional forms, in particular atomically thin films, nanoflakes, and nanowires. Moreover, we study organic nanowires and thin-film coatings.

While liquid-phase exfoliation can be used to produce nanosheets stabilized in polymer solutions, very little is known about the resultant nanosheet size, thickness, or monolayer content. The present study uses semi-quantitative spectroscopic metrics based on extinction, Raman, and photoluminescence (PL) spectroscopy to investigate these parameters for WS<sub>2</sub> nanosheets exfoliated in aqueous poly(vinyl alcohol) (PVA) solutions. By measuring Raman and PL simultaneously, the monolayer content can be tracked via the PL/Raman intensity ratio, while varying the processing conditions. The PL is found to be maximized for a stabilizing polymer concentration of 2 g/L. In addition, the monolayer content can be controlled via the centrifugation conditions, exceeding 5% by mass in some cases. These techniques have allowed us to track the ratio of PL/Raman in a droplet of polymer-stabilized WS<sub>2</sub> nanosheets as the water evaporates during composite formation. No evidence of nanosheet aggregation is found under these conditions although the PL becomes dominated by trion emission as drying proceeds and the balance of doping from PVA/water changes. Finally, bulk PVA/WS<sub>2</sub> composites are produced by freeze drying where >50% of the monolayers remain unaggregated, even at WS<sub>2</sub> volume fractions as high as 10%. This work has been published in *Adv. Funct. Mater.* **26**, 1028–1039 (2016) and is listed as highly cited (i.e., in the top 1% papers in materials science).

Semiconducting TMDs have been applied as the active layer in photo-detectors and solar cells, displaying substantial charge photogeneration yields. However, their large exciton binding energy, which increases with decreasing thickness (number of layers), as well as the strong resonance peaks in the absorption spectra suggest that excitons are the primary photoexcited states. Detailed time-domain studies of the photoexcitation dynamics in TMDs exist mostly for MoS<sub>2</sub>. We used femtosecond optical spectroscopy to study the exciton and charge dynamics following impulsive photoexcitation in few-layer WS<sub>2</sub>. We confirm excitons as the primary photoexcitation species and found that they dissociate into charge pairs with a time constant of about 1.3 ps. The better separation of the spectral features compared to MoS<sub>2</sub> allowed us to resolve a previously undetected process: these charges diffuse through the samples and become trapped at defects, such as flake edges or grain boundaries, causing an appreciable change of their transient absorption spectra. This finding opens the way to further studies of traps in TMD samples with different defect contents. The work has been published in *Nanoscale* **8**, 5428–5434 (2016).

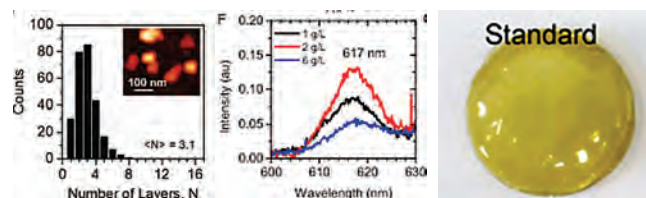
The electronic and photophysical properties of a material depend crucially the electron relaxation behavior. Ionic surfactants, which are widely used to stabilize nanomaterials in dispersions, can drastically alter the nanomaterial's photophysical properties. Here, we used femtosecond optical spectroscopy to study the dynamics of excitons and charges in few-layer flakes of the two-dimensional semiconductor MoS<sub>2</sub>. We compare samples obtained via exfoliation in water with different amounts of adsorbed sodium cholate, obtained by repeated washing of the dried flakes. We find that the femtosecond dynamics is remarkably robust against the surfactant adsorption, with a slight increase of the initial exciton quenching occurring during the first few picoseconds as the only appreciable effect. The work has been published in the *Journal of Nanophotonics* **10**, 012508-1–8 (2016) and was among the top ten downloads of that journal throughout 2016.

We show that gold-decorated MoS<sub>2</sub> flakes are amenable to thiol chemistry by blending them with a cross-linkable thiolated polysiloxane (PMMS). MoS<sub>2</sub> flakes from chemical exfoliation are mostly in the metallic 1T rather than the semiconducting 2H phase. One typically recovers the semiconducting phase by thermally transforming 1T into 2H. Blending MoS<sub>2</sub> into the viscous PMMS has many interesting consequences: PMMS acts as a surfactant and makes MoS<sub>2</sub> dispersible in additional solvents such as chloroform, it makes the 1T and 2H flakes dispersible in the same solvent, enabling transformation in a single step by heating the dispersion, and it prevents the MoS<sub>2</sub> flakes from restacking upon drying, which is a great advantage for all forms of deposition from liquid, including printing. Upon cross-linking, PMMS forms an elastomer of good optical quality, which contains individual, mostly single-layer MoS<sub>2</sub> flakes. These are suitable for saturable absorbers, optical limiters, or strain-tuning of the optical resonances, due to the superior anchoring of the elastomer on the flakes through the gold nanoparticles. Besides the new material combination with good biocompatibility, our findings show that the driving force is the interac-

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**We produced fluorescent polymer/WS<sub>2</sub> composites by direct exfoliation in an aqueous polymer solution.**

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*Figure 2: Fluorescent polymer/WS<sub>2</sub> composites. Left: Thickness histogram of exfoliated WS<sub>2</sub> after centrifugation (inset: AFM image of typical flakes). Centre: Fluorescent spectra of WS<sub>2</sub> dispersions. Right: Photograph of a polymer/WS<sub>2</sub> composite film.*

tion between the thiol groups and the gold nanoparticles. This opens up applications based the anchoring on the gold nanoparticles of thiolated antibodies/antigens for biosensing and electron donor or acceptor molecules for light harvesting. These results, which have been obtained in collaboration with the Laboratory for surface and thin film analysis (F4), have been published in *Nanoscale* **8**, 10016–10020 (2016).

**We produced highly monolayer-enriched dispersions of liquid-exfoliated nanosheets by liquid-cascade centrifugation.**

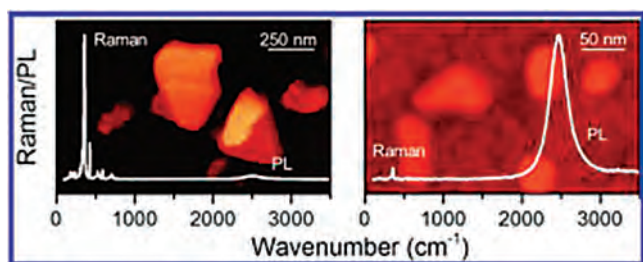


Figure 3: Monolayer-enriched dispersions of WS<sub>2</sub> nanosheets by liquid cascade centrifugation. Left: Raman and PL spectra and AFM image of larger flakes after centrifugation. Right: Raman and PL spectra and AFM image of mostly monolayer flakes after centrifugation.

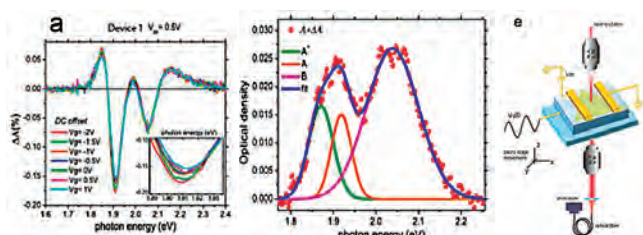


Figure 4: Electro-absorption of monolayer MoS<sub>2</sub>. Left: Scheme of the measurement apparatus consisting of a confocal microscope, tunable laser, and transparent MoS<sub>2</sub> transistor. Centre: Electro-absorption spectra for different DC bias voltages. Right: decomposition of the absorption spectrum in the presence of the electric field into the two excitonic resonances A and B and the trion resonance A<sup>-</sup>.

**Monolayer MoS<sub>2</sub> shows an unprecedentedly strong electro-absorption effect with an unusual field dependence.**

ing are used to investigate the spatial inhomogeneity of solar cell parameters and correlate them with the device's performance. The effect is strongly correlated to the regioregularity of P3HT with highly regioregular P3HT having the largest effect. Our work was published in *Synthetic Metals* **212**, 105–112 (2016).

We have shown that we can control the electric-field-induced local domain growth with a magnetic field. Local bias application by a conducting atomic force microscope tip induced local charged states at the surface of lanthanum strontium manganite single crystals. The piezoelectric contrast observed in these states points to the existence of a local polar state. The induced charged states relax with a characteristic time constant of about 50–100 hours at room temperature. The charge and size of the created structures increase significantly if the induction occurs in a magnetic field. This finding indicates the tendency of manganites towards charge segregation stimulated by the magnetic ordering. These results have been published in *Ferroelectrics* **499**, 143–149 (2016).

Several synthetic routes exist for the production of bulk molybdenum carbides whereas the production of larger quantities of different molybdenum carbide phases in the form of nanowires and nanowire networks is still challenging. Here we report a novel route for the synthesis of molybdenum carbide nanowires by carburisation of Mo<sub>6</sub>S<sub>2</sub>I<sub>8</sub> nanowire bundles. Gram quantities of molybdenum carbide nanowires composed of mainly MoC and Mo<sub>2</sub>C phases were obtained and further reduced to single-phase Mo<sub>2</sub>C nanowires. By controlling the reaction conditions during the transformation, we can modify the ratio between MoC and Mo<sub>2</sub>C phases in nanowires and produce a novel

While liquid exfoliation is a powerful technique to produce defect-free nanosheets in large quantities, its usefulness is limited by broad nanosheet thickness distributions and low monolayer contents. We demonstrated liquid processing techniques, based on iterative centrifugation cascades, which can be designed to achieve either highly efficient nanosheet size-selection and/or monolayer enrichment. We used the resultant size-selected dispersions to establish quantitative metrics to determine monolayer volume fraction, as well as mean nanosheet size and thickness, from standard spectroscopic measurements. Such metrics allowed us to design and optimize centrifugation cascades to enrich liquid exfoliated WS<sub>2</sub> dispersions up to monolayer contents of 75%. Monolayer-rich dispersions show relatively bright photoluminescence with narrow line widths (<35 meV) indicating the high quality of the nanosheets. The enriched dispersions display extinction spectra with distinct features, which also allow the direct estimation of monolayer contents. This work was published in *ACS Nano*, **10**, 1589–1601 (2016) and is listed as highly cited (i.e., in the top 1% of papers in Chemistry).

Signal modulation in optoelectronics is obtained by modulation of either the refractive index or the absorbance by an electric field. However, electro-modulators have not kept up with the miniaturization of other electronic and optical components. Here we show a strong transverse electro-absorption signal in a monolayer of the two-dimensional semiconductor MoS<sub>2</sub>. The electro-absorption spectrum is dominated by an apparent linewidth broadening of around 15% at a modulated voltage of only  $V_{pp} = 0.5$  V. Contrary to known variants of the Stark effect, the broadening increases linearly with the applied field strength and arises from a linear variation of the distance between the strongly overlapping exciton and trion resonances. The achievable modulation depths exceeding 0.1 dB nm<sup>-1</sup> bear the scope for extremely compact, ultrafast, energy-efficient electro-absorption modulators for integrated photonics, including on-chip optical communication. This work has been published in the journal *2D Materials*, **4**, 021005 (2017). Moreover, we filed a UK patent application for the proposed electromodulator device: GB 1600549.8.

We have achieved a remarkable 52% relative increase in power conversion efficiency (PCE) of solar cells embedded with small amounts of MoSI nanowires dispersed in a P3HT:PCBM matrix. We have presented a detailed and systematic investigation of the numerous factors influencing this breakthrough increase. Raman spectroscopy and photocurrent imag-

hybrid inorganic/organic nanomaterial that we identified as molybdenum carbide nanowires densely covered with carbon nanofibres. We used the same approach on nanowire networks and demonstrate a new use of molybdenum carbide in the form of nanowire networks as transparent electrodes. The sheet resistance of such robust and air-stable electrodes is around  $1050 \Omega \text{sq}^{-1}$  at room temperature and their transmittance between 93% and 95% in the range of 200–900 nm. The electrodes are thus suitable for electro-optic applications, especially where high transparency in the UV region is required. These results have been published in *RSC Advances* **6**, 90806–90812 (2016).

We developed a novel and efficient method used to improve the carrier mobilities of poly(3-hexylthiophene) (P3HT)-based organic field-effect transistors by means of nanowire formation. The treatment, termed solvation, consists of depositing a small quantity of a solvent directly on top of a previously deposited semiconducting film, and allowing the solvent to evaporate slowly. Such treatment results in an increase of the saturation mobility by more than one order of magnitude, from  $1.3 \times 10^{-3}$  up to  $3.4 \times 10^{-2} \text{ cm}^2/\text{Vs}$ , while devices preserve their high ON/OFF ratio of similar to  $10^4$ . The atomic force and scanning electron microscopy studies show that solvated P3HT layers develop a network of nanowires, which exhibit an increased degree of structural order, as demonstrated by micro Raman spectroscopy. The time-of-flight photoconductivity studies suggest that higher hole mobility stems from a reduced energy disorder of the transporting states in these structures. These results have been published in *Organic Electronics* **30**, 92–98 (2016).

We investigated the local electronic structure of purified  $\text{Mo}_6\text{S}_{9-x}\text{I}_x$  ( $x = 6, 4.5$ ) nanowires by X-ray absorption and fluorescence spectroscopies. The nanowires are found to be metallic with the density of states altered in both the conduction and the valence band depending on the stoichiometry. First-principle theoretical calculations suggest that the changes can be mainly attributed to the effect of strong Mo-S hybridization in the nanowires. The atomic chain structure of the nanowires is confirmed and the effect of increasing sulphur content is investigated. The results have been published in the *Journal of Electron Spectroscopy and Related Phenomena* **207**, 29–33 (2016).

We investigated the role of zirconium tetrapropoxide (ZTP) and methacrylic acid (MAA), following their combination with sol synthesized from tetraethyl orthosilicate (TEOS) and 3-methacryloxypropyl trimethoxysilane (MAPTMS). The molar content of ZTP was varied between 0.06 and 0.96 and that of MAA between 0.12 and 1.92. The synthesized sols were deposited as coatings on aluminium substrates. The effects of the ageing of sols and the curing of the coatings were examined. The composition of the sol, ageing process and size distribution of the particles, the thermal stability of the sols and coatings, the phase composition and microstructure of the coatings and contact angle of the water drop at the coating surface were all investigated. Comparison of sols, using Fourier transform infrared spectroscopy, confirmed important differences in terms of the presence of Si-O-Zr and chelated ZTP-MAA bonds. The three sols studied differ significantly in their ageing behaviour, as shown by dynamic light scattering. Thermogravimetric analysis and analysis of the vapour side products during the curing process confirmed the effect of sol composition on the mass loss at elevated temperatures. Morphology, phase composition and structure of the coating were analysed with scanning and transmission electron microscopy, atomic force microscopy and X-ray diffraction analysis. The coatings possess a homogeneous and amorphous structure, without the formation of nanoparticles. Synthesized coatings offer high corrosion protection of aluminium under simulated aircraft conditions. This work has been published in *Surface and Coatings Technology* **286**, 388–396 (2016).

Nanowires and nanotubes decorated with platinum nanoparticles are known for their excellent sensing and catalytic properties. However, the decoration of transition-metal dichalcogenide nanotubes can be very complex. We have discovered a simple procedure that enables efficient production and purification of thin bundles of MoSI nanowires decorated with platinum nanoparticles and a simple procedure for direct decoration of  $\text{MoS}_2$  nanotubes. First, we isolated several hundred milligrams of nanowire bundles that were several microns long with average diameters of around 40 nm, and formed a stable dispersion in water without added surfactants. Platinum nanoparticles were directly deposited on the nanowire bundles in a solution at room temperature in a single-step reaction without any additional reducing reagents. A stable and uniform decoration is observed with average particle diameters of around 2 nm and a controllable surface density, covering up to 80% of the nanowire surface. Similar decoration takes place also on  $\text{MoS}_2$  nanotubes dispersed in water. Sulfurization of decorated nanowires was performed, during which platinum nanoparticles aggregated into larger formations, and partial encapsulation of elongated platinum nanorods in the obtained multi-wall  $\text{MoS}_2$  nanotubes is observed. These results are reported in *Materials Letters* **159** (2015) 333–336.

### Soft Matter

In cooperation with Nankai University in China we investigated liquid-crystal alignment at interfaces with thin polymeric walls that are oriented in a direction perpendicular to the glass substrates. The walls are fabricated by a direct laser writing process based on two-photon polymerization. This method provides micro-structured liquid-crystal alignment in practically oblique configurations, which opens up several possibilities for applications in liquid-crystalline optical modulators and spatial light filters, microfluidic units based on liquid crystals, etc. The



results of this work were reported in *Optics Letters* 41, 336 (2016). The described alignment approach is also the main topic of the granted Chinese patent (CN103995394(B), 2016-08-17).

In cooperation with the University of Luxembourg we continued with investigations of the optical properties of 2D arrangements of droplets and shells made of cholesteric liquid crystals. We found that the shells exhibit optical reflection patterns with much better quality than the droplets. We also demonstrated that the addition of a photopolymerizable moiety to such structures results in optical materials exhibiting reversibly changing optical properties even at relatively large mechanical deformations. This makes them very promising for application in authentication tags for the protection of products against imitation. The results were published in *Scientific Reports* 6, 26840 (2016). We also started collaborative investigations of structural and optical properties of cellulose nanocrystalline films (CNCs). We found that films prepared with and without the presence of a shear flow exhibit very different structural quality, while their optical reflective properties are quite similar. The results of this work were reported in *Cellulose* 23, 3601 (2016).

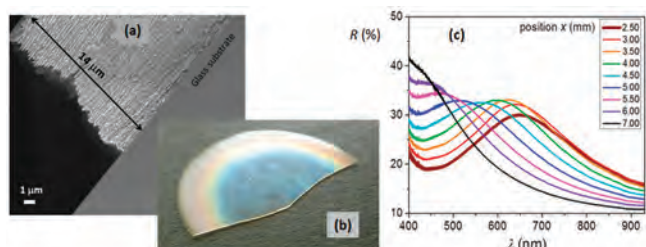


Figure 5: (a) SEM image of cross-sectional plane of cellulose nanocrystalline (CNC) film revealing its periodic microstructure. (b) Photograph of the film showing its iridescent coloration. (c) Diffuse reflectance spectra of the film measured at different distances from the peripheral border.

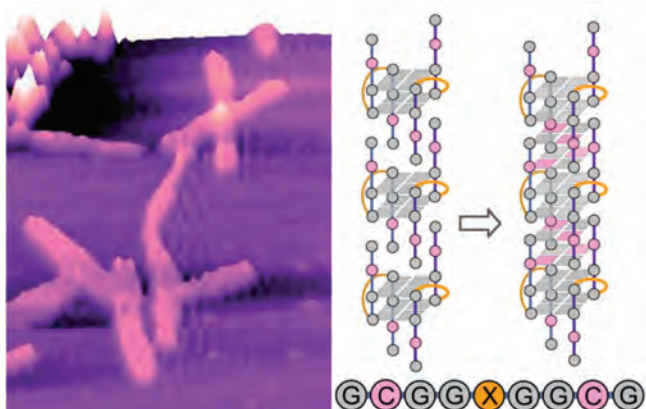


Figure 6: AFM image of G-wires formed on mica surface and bonding scheme of base sequences containing both 5' and 3' GC-ends

**Formation of G4-nanowires from G-rich DNA oligonucleotides on surface of solid substrates was systematically investigated.**

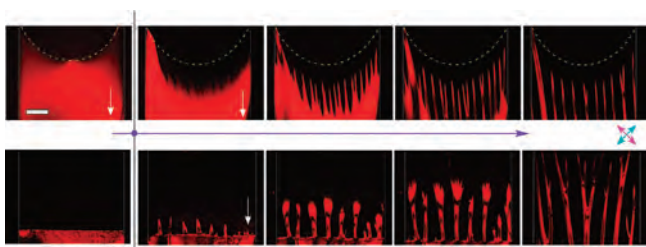


Figure 7: Ferromagnetic nematic spikes at the BF/BuOH isotropic/nematic interface From *Nature Communications* 7, 10394 (2016)

**We have studied field-induced structures in ferromagnetic chiral nematic liquid crystals.**

We performed systematic analyses of the self-assembly of DNA oligonucleotides in drop-cast thin films deposited onto solid substrates. Using AFM imaging, we analyzed a set of guanosine (G)-rich oligonucleotides with GC-termini for their ability to form long G-wires through G:C pairing. We investigated the effects of increasing sequence length, the type of nucleotide in the side loops, and removal of the CG-3' terminus. We found that sequences with adenine in the side loops most readily form G-wires. The role of magnesium as an efficient surface-anchoring ion was also confirmed. These observations were published in *Langmuir* 32, 7056 (2016). We concluded an investigation of the molecular recognition of lipophilic guanosine derivatives in Langmuir films at air-water interfaces. The investigation took place via film balance experiments and Brewster Angle Microscopy (BAM). The results showed that guanosine, despite strong tendency towards self-assembly, interacts with both complementary and noncomplementary liponucleosides. This indicates that  $\pi$ -stacking interactions between the aromatic planes of liponucleoside derivatives probably dominate over hydrogen-bonding interactions. The work is reported in *Biochimica et Biophysica Acta (BBA) - General Subjects*, available on line (2016).

In cooperation with the University of Vienna we continued investigations of holographic micro-patterning in light-sensitive liquid-crystalline elastomers. We examined an unusual effect of destructive interference observed in optical polarization gratings and found that it originates from the strong anisotropy of optical absorbance of the material for recording optical radiation. The results were published in *Optical Materials Express* 6, 961 (2016).

We have extended our studies of the properties of a ferromagnetic phase to the suspensions of magnetic platelets in chiral nematic liquid crystals, called also cholesteric liquid crystals (CLCs). CLCs form a rich variety of configurations and defect structures when confined in layers or droplets. In confined CLCs surface anchoring usually promotes a uniform configuration, which competes with the helical ground state of bulk CLCs. These frustrated structures can be further manipulated by electric and large magnetic fields. In suspensions of magnetic nanoplatelets in CLCs, similarly as in the suspension in nematic liquid crystals, ferromagnetic ordering of the platelets appears, which makes the suspensions sensitive also to small magnetic fields. These ferromagnetic CLCs can be described macroscopically by two coupled order parameters: the director and the magnetization. The coupling is such that a parallel orientation of the order parameters is the most favorable. The director is sensitive to the electric field and its configuration is preferably helical, while the magnetization is sensitive to small magnetic fields and it prefers a homogenous state, so the frustration is inherent already in the bulk. We have studied the field-induced structures of such ferromagnetic CLC confined to a layer with homeotropic (perpendicular) surface anchoring and a thickness of approximately two cholesteric pitches. We used

different combinations of electric and magnetic fields to manipulate the structures. The results of our studies were presented at the International Liquid Crystal Conference (ILCC 2016), Kent, OH, USA, and at the 6<sup>th</sup> Workshop on Liquid Crystals for Photonics, Ljubljana, Slovenia.

In collaboration with the University of Boulder, Colorado, USA we discovered that the suspension of magnetic nanoplatelets in butanol exhibit ferromagnetic ordering. This is the first experimental realization of a ferromagnetic ferrofluid. Its zero-field magnetization produces distinctive magnetic self-interaction effects, including liquid crystal textures of fluid block domains arranged in closed flux loops, and makes this phase highly sensitive, with it dramatically changing shape even in the Earth's magnetic field (*Nature Communications* 7, 10394 (2016)).

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**Ferromagnetic ferrofluid has been realized in the dense suspension of magnetic nanoplatelets in 1-butanol.**

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### Nonlinear optics

In the Nonlinear Optics Laboratory we study new materials and their interaction with laser light. In cooperation with North Carolina State University, Raleigh, USA, we study new concepts of compact light sources on the basis of nonlinear optical conversion of existing lasers into the short wavelengths spectral regions where lasers are not yet available. AlGaIn grown by metalorganic chemical vapor deposition (MOCVD) has a great potential for optoelectronic devices emitting and detecting light in the ultraviolet spectrum. It is also transparent for THz frequencies, making it interesting for new THz applications.

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 alternating sign of the nonlinear coefficient that allows quasi phase matching.

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**AlGaIn waveguides in various geometries that allow for phase-matched second-harmonic generation into the UV spectral region are produced and investigated. Other nonlinear optical applications of AlIn are also studied.**

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### Biomedical optics

We have continued with the development of novel biomedical applications based on pulsed photo-thermal radiometry (PPTR). By combining such non-contact measurements of laser-induced radiometric transients with diffuse reflectance spectroscopy and inverse analysis utilizing a numerical model of light transport in strongly scattering biological tissue, we have developed a unique approach for the noninvasive assessment of structure and composition of human skin *in vivo*.

The same experimental and analysis approach (multi-dimensional nonlinear optimization) in conjunction with an analytical model of bruising in human skin was also adapted for an assessment of the hemoglobin mass diffusion coefficient and biochemical decomposition rate in incidental traumatic bruises (hematomas). The improved understanding of bruise dynamics and the developed methodology could enable a significantly more accurate and reliable determination of the time of injury in forensic science in the near future.

Both studies are supported by an equipment loan from Fotona, d.o.o., Ljubljana.

We have participated in the development of novel co-doped inorganic nanoparticles which exhibit so-called up-conversion fluorescence (e.g., Yb<sup>3+</sup>, Tm<sup>3+</sup>:NaYF<sub>4</sub>). By optimization of their size and fluorescence quantum yield, such nanoparticles would exhibit great potential for diagnostic imaging in medicine and enable new approaches to cell-specific therapy, especially for cancer. We have studied their optical properties in relation to synthesis approach, and dissolution kinetics in aqueous media under varying conditions, which is critically important from the point of view of biocompatibility and suitability for biomedical applications. (Collaboration with Department for Materials Synthesis, IJS; Department for Inorganic Chemistry and Technology, IJS; and Medical University of Graz, Austria)

In a detailed simulation study, employing our custom three-dimensional model of light transport in spatially heterogeneous biological organs (Monte Carlo), we have analyzed the influence of the assumed scattering phase function (e.g., Henyey-Greenstein, modified Henyey-Greenstein, or Mie) on the assessment of tissue properties and morphology in hyperspectral imaging using customary protocols.

The same light-transport model was also applied to simulations of the interactions between intense laser pulses and cutaneous blood vessels containing particular nanostructures of different sizes. These nanostructures were successfully engineered from animal erythrocytes and contained FDA-approved infrared-absorbing dye (indocyanine green). The aim of the project is to derive biocompatible and safe nanoprobes for diagnostic imaging in small

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**By combining pulsed photothermal radiometry and diffuse reflectance spectroscopy with inverse analysis based on a numerical model of light transport in biological tissue, we have developed a unique approach for the quantitative assessment of structure and composition of human skin *in vivo*.**

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animals and possibly also human patients. (Collaboration with University of California at Riverside and Beckman Laser Institute and Medical Clinic, University of California at Irvine, USA).

### Colloidal systems

Microfluidic research of colloidal systems was conducted in close collaboration with Laboratory of Experimental Soft Matter at Faculty of Mathematics and Physics, University of Ljubljana and Department of Condensed Matter Physics (F5). The experiments were performed on magneto-optical tweezers and other laboratory equipment that was developed and produced specifically for our research. The microfluidic research of soft matter included the production of hybrid colloidal particles with laser direct imaging (LDI), an investigation of magnetic colloidal vortices, flow vortices in microfluidic channels, opto-thermal microfluidic pump and investigations of anomalous diffusion in anisotropic fluids.

Laser direct imaging is a maskless lithographic method that enables the fast and precise production of hybrid microstructures. We have shown the advantages of this method by manufacturing microparticles of arbitrary shapes, sizes, and thicknesses functionalised with a variety of materials, for example, fluorescent microbeads or superparamagnetic spheres. The variety of particles gives rise to different colloidal phenomena, the particles are suitable for studying interparticle interactions and can be used in microfluidic devices. We concluded the research on interaction of superparamagnetic beads in a precessing external magnetic field. Within a range of field frequencies, we observed dynamic large-scale structures such as ordered phases composed of precessing chains, ribbons, and rotating fluidic vortices. The results were published in *Applied Physics Express* and *Langmuir*.

In collaboration with the Institute of Biophysics, Medical Faculty, University of Ljubljana, and Group of Soft and Partially Ordered Matter, Faculty of Mathematics and Physics, we investigated fluid flows in elongated side-channels of microfluidic devices. Detailed experimental observations, combined with theoretical analysis and numerical simulations have shown the existence of vortices that appear at large channel aspect ratios. The position of the first vortex depends exponentially with the increasing aspect ratio, whereas below the critical values, the flow decreases exponentially from the cavity entrance. The results of the research were published in *Microfluidics and Nanofluidics*.

We demonstrated a working microfluidic micropump that was based on thermo-viscous fluid pumping. Due to local changes in viscosity and local thermal expansion, a rapidly moving heated area can lead to relatively large fluid flows. We manufactured a series of microheaters, developed the steering electronics and tested its efficiency by following the included tracer particles. Rapidly varying thermal gradients were also used for the manipulation of individual microparticles in so-called opto-thermal tweezers. The high-temperature areas were created by absorbing IR laser light and the successful particle manipulation was shown on micron- and submicron-sized particles. The experiments were made as a part of Jošt Stergar's bachelor thesis.

We also investigated the motion of microparticles in anisotropic fluids, which included liquid crystals. Due to the anisotropic nature of the matter, diffusion of the particles depends on the direction of motion giving two distinct diffusion coefficients: parallel and perpendicular to the director. We studied diffusion in recently discovered ferromagnetic liquid crystals, where the diffusion is influenced by the fluctuations, which in turn can be influenced by external magnetic fields. The diffusion coefficients were thus measured as a function of the magnetic field and we have shown that a reduction of diffusion appears along with subdiffusion. We conclude that the observed subdiffusion is a result of local heterogeneities in the sample. The research was a part of a bachelor thesis, which was successfully defended by Hana Majaron.

### Some outstanding publications in the past year

1. Vaskivskiy, Igor, Mihailović, Ian, Brazovskii, Serguei, Gospodarič, Jan, Mertelj, Tomaž, Svetin, Damjan, Šutar, Petra, Mihailović, Dragan. Fast electronic resistance switching involving hidden charge density wave states. *Nature communications*, ISSN 2041-1723, 2016, vol. 7, str. 11442 -1-11442 -5, doi: 10.1038/ncomms11442. [COBISS.SI-ID 29594919]
2. Madan, Ivan, Kušar, Primož, Baranov, Vladimir V., Lu-Dac, Mathieu, Kabanov, Viktor V., Mertelj, Tomaž, Mihailović, Dragan. Real-time measurement of the emergence of superconducting order in a high-temperature superconductor. *Physical review. B, Condensed matter and materials physics*, ISSN 1098-0121, 2016, vol. 93, no. 22, str. 224520-1-224520-8, doi: 10.1103/PhysRevB.93.224520. [COBISS.SI-ID 29645351]
3. Ličen, Matjaž, Majaron, Boris, Noh, Junghyun, Schütz, C., Bergström, Lennart, Lagerwall, Jan P. F., Drevenšek Olenik, Irena. Correlation between structural properties and iridescent colors of cellulose nanocrystalline films. *Cellulose*, ISSN 0969-0239, 2016, vol. 23, iss. 6, str. 3601-3609, ilustr., doi: 10.1007/s10570-016-1066-z.

4. Troha, Tinkara, Drevenšek Olenik, Irena, Webba Da Silva, Mateus, Spindler, Lea. Surface-adsorbed long G-quadruplex nanowires formed by G:C linkages. *Langmuir*, ISSN 0743-7463, 2016, vol. 32, iss. 28, str. 7056-7063, ilustr., doi: 10.1021/acs.langmuir.6b01222
5. Ji, Zhichao, Zhang, Xinzheng, Shi, Bin, Li, Wei, Luo, Weiwei, Drevenšek Olenik, Irena, Wu, Qiang, Xu, Jingjun. Compartmentalized liquid crystal alignment induced by sparse polymer ribbons with surface relief gratings. *Optics letters*, ISSN 0146-9592, 2016, vol. 41, iss. 2, str. 336-339, ilustr., doi: 10.1364/OL.41.000336
6. Geng, Yong, Noh, Junghyun, Drevenšek Olenik, Irena, Rupp, Romano A., Lenzini, Gabriele, Lagerwall, Jan P. F. High-fidelity spherical cholesteric liquid crystal Bragg reflectors generating unclonable patterns for secure authentication. *Scientific reports*, ISSN 2045-2322, 2016, vol. 6, art. no. 26840, 9 str., ilustr., doi: 10.1038/srep26840.
7. Lisjak, Darja, Plohl, Olivija, Vidmar, Janja, Majaron, Boris, Ponikvar-Svet, Maja. Dissolution mechanism of upconverting  $\text{AYF}_4:\text{Yb,Tm}$  (A = Na or K) nanoparticles in aqueous media. *Langmuir*, ISSN 0743-7463, 2016, vol. 32, no. 32, str. 8222-8229, doi: 10.1021/acs.langmuir.6b02675. [COBISS.SI-ID 29679655]
8. Shuai, M., Mertelj, Alenka, Lisjak, Darja, Čopič, Martin, et al. Spontaneous liquid crystal and ferromagnetic ordering of colloidal magnetic nanoplate. *Nature communications*, ISSN 2041-1723, 2016, vol. 7, str. 10394-1-10394-8, doi: 10.1038/ncomms10394. [COBISS.SI-ID 29253927]

### Some outstanding publications in the year 2015

1. Madan, Ivan, Kurosawa, T., Toda, Y., Oda, Migaku, Mertelj, Tomaž, Mihailović, Dragan. Evidence for carrier localization in the pseudogap state of cuprate superconductors from coherent quench experiments. *Nature communications*, ISSN 2041-1723, 2015, vol. 6, str. 6958-1-6958-6, doi: 10.1038/ncomms7958. [COBISS.SI-ID 28758311]
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3. Shumilin, A. V., Kabanov, Viktor V.. Kinetic equations for hopping transport and spin relaxation in a random magnetic field. *Physical review. B, Condensed matter and materials physics*, ISSN 1098-0121, 2015, vol. 92, no. 1, str. 041206-1-041206-15, doi: 10.1103/PhysRevB.92.014206. [COBISS.SI-ID 28747047]
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### Some outstanding publications in the year 2014

1. 1. Stojchevska, Ljupka, Vaskivskiy, Igor, Mertelj, Tomaž, Kušar, Primož, Svetin, Damjan, Brazovskii, Serguei, Mihailović, Dragan. Ultrafast switching to a stable hidden quantum state in an electronic crystal. *Science*, ISSN 0036-8075, 2014, vol. 344, no. 6180, str. 177-180, doi: 10.1126/science.1241591. [COBISS.SI-ID 27627303]
2. 2. Madan, Ivan, Kurosawa, T., Toda, Y., Oda, Migaku, Mertelj, Tomaž, Kušar, Primož, Mihailović, Dragan. Separating pairing from quantum phase coherence dynamics above the superconducting transition

- by femtosecond spectroscopy. *Scientific reports*, ISSN 2045-2322, 2014, vol. 4, str. 05656-1-05656-5, doi: 10.1038/srep05656. [COBISS.SI-ID 27876647]
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  4. 4. Tašič, Blaž, Mrzel, Aleš, Huskić, Miroslav, Zhang, Xinzhen, Drevenšek Olenik, Irena. 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, str. 26396-26401, ilustr. <http://pubs.acs.org/doi/abs/10.1021/jp508412w>, doi: 10.1021/jp508412w. [COBISS.SI-ID 2746468]
  5. 4. Čoga, Lucija, Masiero, Stefano, Drevenšek Olenik, Irena. Lamellar versus compact self-assembly of lipoguanosine derivatives in thin surface films. *Colloids and surfaces. B, Biointerfaces*, ISSN 0927-7765. [Print ed.], 2014, vol. 121, str. 114-121, ilustr. <http://www.sciencedirect.com/science/article/pii/S0927776514002732#>, doi: 10.1016/j.colsurfb.2014.05.038. [COBISS.SI-ID 2686564]
  6. 5. Mertelj, Alenka, Osterman, Natan, Lisjak, Darja, Čopič, Martin. Magneto-optic and converse magneto-electric effects in a ferromagnetic liquid crystal. *Soft matter*, ISSN 1744-683X, 2014, vol. 10, no. 45, str. 9065-9072, doi:10.1039/C4SM01625D. [COBISS.SI-ID 28078119]
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  8. 7. Buh, Jože, Kovič, Andrej, Mrzel, Aleš, Jagličič, Zvonko, Jesih, Adolf, Mihailović, Dragan. Template synthesis of single-phase  $\delta$ -MoN superconducting nanowires. *Nanotechnology*, ISSN 0957-4484, 2014, vol. 25, no. 2, str. 025601-1-025601-6, doi: 10.1088/0957-4484/25/2/025601. [COBISS.SI-ID 27331623]
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## Organization of conferences, congresses and meetings

1. Nonequilibrium Phenomena in Quantum Systems, Ambrož pod Krvavcem, Slovenia, organizers, 17.12.-21.12.2016
2. Flatlands beyond Graphene 2016, Bled, Slovenia, organizers, 4.7.-8.7.2016

## Patents granted

1. Xinzhen Zhang, Jingjun Xu, Wei Li, Irena Drevenšek Olenik, Wei Cui, Bin Shi, Zhenhua Wang, Qiang Wu, Yongfa Kong, Micro/nano region liquid crystal alignment method and system thereof based on laser direct writing, CN103995394 (B), Chinese Patent Office, 17. 08. 2016.
2. Andrej Kovič, Adolf Jesih, Aleš Mrzel, Process for the synthesis of the molybdenum carbide in the form of quasi-one-dimensional structures, that is, nano-wires, micro-wires, nano-strips and micro-strips, SI24925 (A), Slovenian Intellectual Property Office, 31. 08. 2016.
3. Igor Vaskivskiy, Dragan Mihailović, Ian Mihailović, Switchable macroscopic quantum state devices and methods for their operation, SI24776 (A), Slovenian Intellectual Property Office, 29. 01. 2016.
4. Matjaž Lukač, Zdenko Vižintin, Boris Cenčič, Method for lightening or eradicating pigments in human skin, US9254174 (B2), US Patent Office, 09. 02. 2016.

## INTERNATIONAL PROJECTS

1. Kimberly-Clark - Development of LCD Shutter in the Year 2016  
Prof. Martin Čopič  
Kimberly-clark
2. Spectra Measurements XANES/EXAFS; Extend Existing Work and Include Completing the Data Analysis and Writing s Paper for Submission to a Referred Journal  
Dr. Steven Daniel Conradson  
Areva Mining And Front-end Bg
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. COST MP1205; Advances in Optofluidics: Integration of Optical Control and Photonics with Microfluidics  
Dr. Natan Osterman  
Cost Office
6. COST MP1302; NanoSpectroscopy

- Prof. Christoph Gadermaier  
Cost Office
- MPNS COST MP1201: Nanoscale Superconductivity: Novel Functionalities through Optimized Confinement of Condensate and Fields - NanoSC - COST  
Prof. Viktor Kabanov  
Cost Office
  - COST BM 1205: Biomedicine and Molecular Biosciences  
Prof. Boris Majaron  
Cost Office
  - H2020 - MagNem; Hydrodynamics of Ferromagnetic Nematic Liquid Crystals  
Asst. Prof. Alenka Mertelj  
European Commission
  - JET Campaigns-JET1-FU, EUROFUSION  
Dr. Natan Osterman  
European Commission
  - Medium Size Tokamak Campaigns-MST1-FU,  
Dr. Natan Osterman  
European Commission
  - Neutron Polarizers based on Polymer-nanoparticle Composites  
Prof. Martin Čopič  
Slovenian Research Agency
  - Evaluation of Tissue Depth Characterization in Vivo Using Photothermal Radiometry by Co-registration with Alternative Novel Approaches  
Prof. Boris Majaron  
Slovenian Research Agency
  - Growth and Characterization of Functional 2D Materials based on Graphene and Dichalcogenides  
Asst. Prof. Tomaž Mertelj  
Slovenian Research Agency
  - Photo-Stimulated Phenomena and Dynamical States in the Vicinity of the Phase Transition  
Prof. Viktor Kabanov  
Slovenian Research Agency

## RESEARCH PROGRAMS

- Theory of the condensed matter and statistical physics  
Prof. Janez Bonča
- Theoretical physics of nuclei, particles and fields  
Prof. Sveltana Fajfer
- Light and Matter  
Prof. Martin Čopič
- Medical physics  
Dr. Matija Milanič
- Dynamics of complex nano-systems  
Prof. Dragan Dragoljub Mihailović

## R & D GRANTS AND CONTRACTS

- Thermophoretic guidance, accumulation and sorting of biomolecules in microfluidic devices  
Dr. Natan Osterman
- Ultrafast memory devices by molecular beam epitaxy  
Prof. Dragan Dragoljub Mihailović
- Optimization strategies in biological and artificial microfluidic systems  
Dr. Mojca Vilfan
- Symmetry breaking in real time  
Prof. Dragan Dragoljub Mihailović
- Irradiation and Analysis of Nano SiC Samples  
Miloš Borovšak, B. Sc.  
National Nuclear Research Center

## VISITORS FROM ABROAD

- Dr. Silvia Marchesan, Università degli Studi di Trieste, Trieste Italy, 18.1.-22.1.2016
- Dr. Venera F. Nasretdinova, Institute of Radioengineering and Electronics of the Russian Academy of Science, Moscow, Russia, 1.1.-21.1.2016
- Dr. Yaroslav Gerasimenko, Lebedev Physical Institute of the Russian Academy of Science, Moscow, Russia, 1.1.-21.1.2016
- Prof. dr. Steven Daniel Conradson, Institut "Jožef Stefan", Ljubljana, Slovenia, 27.5.-31.5.2016
- Dr. Nataša Vujičić, Institut za Fiziku, Zagreb, Croatia, 31.5.2016
- Dr. Péter Salamon, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Budapest, Hungary, 12.6.-8.7.2016
- Maksim Litskevich, Maxim Bryzgalov, Alexei Shupletcov, P. N. Lebedev Physical Institute of the Russian Academy of Sciences in Moscow Institute of Physics and Technology, Moscow, Russia, 15.7.-20.8.2017
- Dr. Anna Pogrebna, Spectroscopy of Solids and Interfaces, Institute of Molecules and Materials (IMM) Radboud University Nijmegen, Netherlands, 16.9.-1.10.2016
- Dr. Fabio Miletto Granozio, CNR-SPIN, Naples, Italy, 27.9.2016
- Prof. dr. Juergen Klepp, University of Vienna, Vienna, Austria, 7.10.-11.10.2016
- Dr. Yoshiaki Uchida, Department of Materials Engineering Science, Graduate School of Engineering Science Osaka University, Osaka, Japan, 2.11.-8.11.2016
- Dr. Sunil Kumar, Department of Physics, Indian Institute of Technology (IIT), Delhi, India, 11.12.-15.12.2016
- Sanje Fenkart, University of Vienna, Vienna, Austria, 19.12.-20.12.2016

## STAFF

### Researchers

- Dr. Steven Daniel Conradson
  - Prof. Martin Čopič\*
  - Prof. Irena Drevenšek Olenik\*
  - Prof. Christoph Gadermaier
  - Prof. Viktor Kabanov
  - Dr. Matjaž Lukač\*
  - Prof. Boris Majaron
  - Dr. Marko Marinček\*, left 01.02.16
  - Asst. Prof. Alenka Mertelj
  - Asst. Prof. Tomaž Mertelj
  - Prof. Dragan Dragoljub Mihailović, Head
  - Dr. Matija Milanič
  - Dr. Aleš Mrzel
  - Dr. Natan Osterman\*
  - Dr. Nerea Sebastián Ugarteche
  - Asst. Prof. Lea Spindler\*
  - Dr. Mojca Vilfan
  - Prof. Marko Zgonik\*
- ### Postdoctoral associates
- Dr. Jože Buh, left 01.09.16
  - Dr. Luka Cmok
  - Dr. Ivan Madan, left 01.09.16
  - Dr. Ivan Madan, left 01.10.16
  - Dr. Venera Nasretdinova, left 01.09.16
  - Dr. Andrej Petelin
  - Dr. Peter Rodič

- Dr. Anastasia Samodurova
  - Dr. Ljupka Stojčevska Malbašić
  - Dr. Jure Strle
  - Dr. Igor Vaskivskiy, left 01.09.16
- ### Postgraduates
- Miloš Borovšak, B. Sc., left 01.08.16
  - Tetiana Borzda
  - Andrej Kranjec, B. Sc.
  - Matjaž Ličen, B. Sc.
  - Luca Moretti, B. Sc.
  - Matej Prijatelj, B. Sc.
  - Jan Ravnik, B. Sc.
  - Victor Vega Mayoral, B. Sc., left 01.10.16
  - Dr. Daniele Vella
  - Nina Verdell, B. Sc.
  - Dr. Luka Vidovič\*
- ### Technical officers
- Damjan Svetin, B. Sc.
  - Petra Šutar, B. Sc.
- ### Technical and administrative staff
- Sabina Cintauer, B. Sc.
  - Martina Knavs, B. Sc.
  - Janja Milivojevič

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

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  38. Victor Vega Mayoral, Claudia Backes, Damien Hanlon, Umar Khan, Zahra Gholamvand, Maria O'Brien, Georg S. Duesberg, Christoph Gadermaier, Jonathan N. Coleman, "Photoluminescence from liquid-exfoliated WS<sub>2</sub> monomers in poly(vinyl alcohol) polymer composites", *Adv. funct. mater.*, vol. 26, issue 7, pp.1028-1039, 2016.
  39. Victor Vega Mayoral *et al.* (12 authors), "Exciton and charge carrier dynamics in few-layer WS<sub>2</sub>", *Nanoscale*, vol. 8, no. 10, pp. 5428-5434, 2016.
  40. Damjan Vengust, Jan Ravnik, Aleš Mrzel, Mojca Vilfan, "Molybdenum carbide nanowires: facile synthesis, a new hybrid phase and their use as transparent electrodes", *RSC advances*, vol. 6, no. 93, pp. 90806-90812, 2016.
  41. Gleb Varyasov, Katsuhiko Matsumoto, Rika Hagiwara, "Homoleptic octahedral coordination of CH<sub>3</sub>CN to Mg<sup>2+</sup> in the Mg[N(SO<sub>2</sub>CF<sub>3</sub>)<sub>2</sub>]<sub>2</sub>-CH<sub>3</sub>CN system", *Dalton trans. (2003)*, vol. 45, no. 7, str. 2810-2813, 2016.
  42. Eduard Westphal, Hugo Gallardo, Giovanni Finoto Caramori, Nerea Sebastián Ugarteche, Tamba Maria-Gabriela, Alexey Eremin, Susumu Kawauchi, Marko Prehm, Carsten Tschierske, "Polar order and symmetry breaking at the boundary between bent-core and rodlike molecular forms: when 4-cyanoresorcinol meets the carboxilane end group", *Chemistry (Weinh.)*, vol. 22, no. 24, pp. 8181-8197, 2016.
  43. Anna Zimina, Igor Vilfan, Daniel Vrbanič, Valeria Nicolosi, David Batchelor, Ralph Steininger, Dragan Mihailović, "Electronic structure of purified Mo<sub>6</sub>S<sub>(9-x)</sub>I<sub>x</sub> nanowires studied by X-ray spectroscopy", *J. electron spectrosc. relat. phenom.*, vol. 207, pp. 29-33, 2016.

## REVIEW ARTICLE

1. Claudio Giannetti, Massimo Capone, Daniele Fausti, Michele Fabrizio, Fulvio Parmigiani, Dragan Mihailović, "Ultrafast optical spectroscopy of strongly correlated materials and high-temperature superconductors: a non-equilibrium approach", *Adv. Phys.*, vol. 65, no. 2, pp. 58-238, 2016.

## PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

1. Isabella Avigo, Igor Vaskivskiy, Manuel Ligges, Matthias Kalläne, Kai Rossnagel, Ljupka Stojchevska, Dragan Mihailović, "Accessing and probing of the photo-induced hidden state in 1T – TaS<sub>2</sub> with time- and angle-resolved photoemission spectroscopy", In: *Spintronics IX: September 26, 2016, San Diego, California, United State*, (Proceedings of SPIE, vol. 9931), pp. 99313V-1-1-99313V-8.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Aysen Kaya, Matejka Podlogar, Damjan Vengust, Damjan Svetin, Süleyman Kahraman, Aleksander Rečnik, Slavko Bernik, "Hydrothermal

growth of doped ZnO films on amorphous substrates", In: *Conference proceedings 2016*, 52nd International Conference on Microelectronics, Devices and Materials and the Workshop on Biosensors and Microfluidics, September 28 - 30 2016, Ankaran, Slovenia, pp. 37-42.

2. Matija Milanič, Boris Majaron, "Influence of the scattering phase function in numerical modeling of hyperspectral imaging", In: *Optical interactions with tissue and cells XXVII: 13-18 February, San Francisco California, United States*, (Proceedings of SPIE, vol. 9706), (Progress in biomedical optics and imagins, vol. 1, no. 1), pp. 97060Z-1-97060Z-13.

## PATENT

1. Xinzhen Zhang, Jingjun Xu, Wei Li, Irena Drevenšek Olenik, Wei Cui, Bin Shi, Zhenhua Wang, Qiang Wu, Yongfa Kong, *Micro/nano region liquid crystal alignment method and system thereof based on laser direct writing*, CN103995394 (B), Chinese Patent Office, 17. 08. 2016.
2. Igor Vaskivskiy, Dragan Mihailović, Ian Mihailović, *Switchable macroscopic quantum state devices and methods for their operation*, SI24776 (A), Urad RS za intelektualno lastnino, 29. 01. 2016.
3. Matjaž Lukač, Zdenko Vižintin, Boris Cenčič, *Method for lightening or eradicating pigments in human skin*, US9254174 (B2), US Patent Office, 09. 02. 2016.
4. Andrej Kovič, Adolf Jesih, Aleš Mrzel, *Process for the synthesis of the molybdenum carbide in the form of quasi-one-dimensional structures, that is, nano-wires, micro-wires, nano-strips and micro-strips*, SI24925 (A), Urad RS za intelektualno lastnino, 31. 08. 2016.

## MENTORING

1. Víctor Vega Mayoral, *Photophysics of transition metal dichalcogenides obtained from liquid phase exfoliation*: doctoral dissertation, Ljubljana, 2016 (mentor Christoph Gadermaier).
2. Daniele Vella, *Photophysics of atomically thin MoS<sub>2</sub> devices*: doctoral dissertation, Ljubljana, 2016 (mentor Christoph Gadermaier).
3. Luka Cmok, *Dynamics of swollen liquid-crystal elastomers*: doctoral dissertation, Ljubljana, 2016 (mentor Martin Čopič).
4. Nevena Čelič, *The influence of MoSI nanowires on the efficiency of P3HT:PCBM solar cells*: doctoral dissertation, Ljubljana, 2016 (mentor Dragan D. Mihailović).
5. Sabina Hrašan, *The impact of noise to production and education process*: master's thesis, Ljubljana, 2016 (mentor Nataša Vujica Herzog; co-mentor Lea Spindler).
6. Jan Fišer, *Formation and transfer of metallic nano-droplets to a substrate by means of femtosecond laser pulses*: master's thesis, Ljubljana, 2016 (mentor Tomaž Mertelj).
7. Jan Gospodarič, *Broadband spectral response of the hidden state in 1T-TaS<sub>2</sub>*: master's thesis, Ljubljana, 2016 (mentor Tomaž Mertelj).
8. Hana Majaron, *Anisotropic diffusion of microspheres in ferromagnetic liquid crystal*: master's thesis, Ljubljana, 2016 (mentor Alenka Mertelj; co-mentor Mojca Vilfan).
9. Jan Ravnik, *Investigation of the phase transition to the hidden quantum state on femtosecond timescale*: master's thesis, Ljubljana, 2016 (mentor Dragan D. Mihailović; co-mentor Igor Vaskivskiy).
10. Jošt Stergar, *Photothermal manipulation of individual submicron particle*: master's thesis, Ljubljana, 2016 (mentor Natan Osterman).
11. Peter Šušnjar, *A source of extreme ultraviolet light based on high harmonic generation in noble gases*: master's thesis, Ljubljana, 2016 (mentor Irena Drevenšek Olenik; co-mentor Thomas Udem).
12. Nina Verdel, *Silicon Photomultiplier as Cherenkov light sensor in Time-of-Flight Positron Emission Tomography*: master's thesis, Ljubljana, 2016 (mentor Peter Križan; co-mentor Rok Dolenc).





# 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*

Our continuing research in reactor physics was directed towards the development of novel methods for research and power reactor analysis. Preparations are on-going for an experimental campaign at the TRIGA reactor in collaboration with colleagues from CEA – Cadarache, which is planned for 2017. The aim of the experimental campaign is a study of fission chambers with alternative fissile coating materials – neptunium and plutonium. Preliminary calculations of the fission chamber’s response in relation to the position in the reactor core, the control rod positions, the type of fissile coating and the use of transmission filters (cadmium, gadolinium and boron) have been carried out. In collaboration with colleagues from CEA – Cadarache and the JSI Department of Low and Medium Energy Physics and the Experimental Particle Physics Department, an experimental campaign was performed, the aim of which was the characterization of the gamma fields in the TRIGA reactor through measurements using thermoluminescent and optically stimulated luminescent dosimeter detectors (TLD, OSLD), RadFET detectors, a scintillation spectrometer and fission and ionization chambers. The results of the experimental campaign will serve for the validation of Monte Carlo calculations using a two-step method, under development at the Reactor Physics Department, which enables transport calculations of prompt and delayed gamma rays, emitted by radioactive fission and activation products in the reactor. We have recently shown experimentally that the delayed contribution to the total gamma field is significant. In the field of theoretical reactor physics we proposed and developed a method for the calculation of the angular neutron flux. In the framework of the international NATO Science for Peace and Security research project Engineering Silicon Carbide for Enhanced Border and Ports Security we have commenced the development of silicon-carbide-based neutron detectors, applicable for fissile material detection.

We continued international collaboration within the framework of the OECD/NEA coordinated WPEC Subgroup-41. The main objective of the SG-41 is improvement of nuclear data for  $^{241}\text{Am}$  and  $^{237}\text{Np}$ . In 2016 we analysed thermal neutron capture cross sections in  $^{241}\text{Am}$  and  $^{237}\text{Np}$  and their influence on integral parameters. The methodology of activation analysis of measurement in reactor neutron spectra has been upgraded for the case of low-energy resonances and/or bound states as a function of the spectral ratio.

Within the framework of the European CHANDA project we were involved in the process of improving nuclear data for the accelerator-driven reactor MYRRHA, a Generation IV concept. For materials and reaction which have a significant influence on the uncertainty of integral parameters and for which improvement of nuclear data would contribute most to a reduction of the overall uncertainty of the integral parameters, evaluated nuclear data libraries were compared with the available experimental data. The nuclear data libraries were also tested on other integral benchmark experiments, which have sensitivity profiles similar to MYRRHA. Recommendations for re-evaluations and the planning of new experiments is currently under way.

Researchers from the Reactor Physics Department provided technical support for the safe operation of the Krško nuclear power plant (NPP) in 2016. We have independently confirmed nuclear design calculations for the fuel cycle 29 and performed start-up tests after the fuel reloading. A neutron dose rate at several different positions throughout the reactor building has been determined with the MCNP code. Analysis was needed to verify the relocation of the electronic modules for DSM vibration monitoring of the ventilation units at locations with a lower neutron radiation. It is suspected that the reason for DSM modules’ failure is an exposure to high neutron radiation. The neutron dose rate at the new location is 20–40 times lower than at the old locations, confirming the



Head:  
Asst. Prof. Luka Snoj

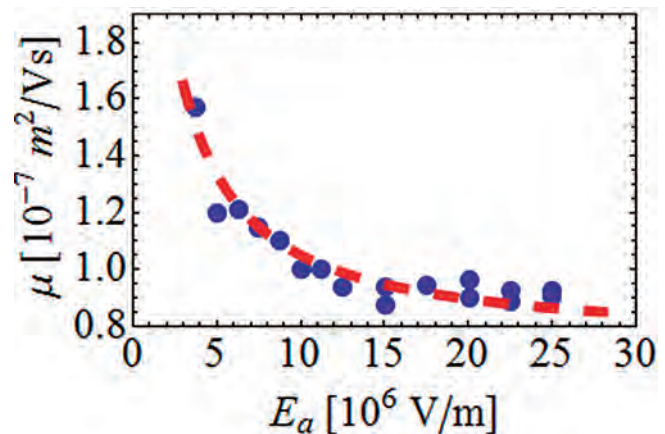


Figure 1: Comparison of the calculated negative hole mobility (dashes) using the bias independent effective hole mobility  $\mu_{\text{eff}} = 2.12 \times 10^{-7} \text{ m}^2/\text{Vs}$  and the linearly increasing electric field at the hole injecting interface on  $E_a$  to the time-of-flight measurements in an 8300-nm-thick layer of PTB7 organic (solid points). The data are adapted from Fig. 1 (b) of Ebenhoch et al., *Org. Electron.* 22 (2015) 62.

suitability of the modification. As an authorized expert organization in the field of radiation and nuclear safety, we have finalized an independent expertise on the Krško NPP reload safety evaluation for cycle 29.

In the field of **plasma physics** we have continued our collaboration in two projects under the EUROfusion flag in 2016. In the project WP15-MST2-14 we have been developing a new probe head for the three EUROfusion MST



Figure 2: Photorealistic schematic of the TRIGA reactor where the core, graphite reflector and ex-core detectors are depicted.

type tokamaks together with Austrian, Italian and Danish researchers. During 2016 the prototypes of the designed probe head parts were tested in the environment of the Linear Magnetized Plasma Device (LMPD) in our department's Laboratory for Plasma Physics. As a part of the project we also began preparing the bases for calculations of the thermal heat load on the probe head. We were again taking part in measurements on the EUROfusion experiments WP15-MST1-AUG15/TCV15-2.2-3 dealing with the filamentary transport in the SOL of tokamaks AUG and TCV. Our task was evaluating the signals from the Langmuir probes. We continued to work together with our colleagues from the University St. Kliment Ohridski from Sofia on the development of the plasma parameter measurements in strongly magnetized plasmas using Langmuir probes. We have made a series of measurements in the LMPD using a triple Langmuir probe in a strong magnetic field and confirmed our theoretical predictions. We have continued our collaboration on the further development of electron-screening probes with the University of Innsbruck. We worked on an improved design of the bunker probe named the bullet probe, but the first results are not as convincing as at the former. We made progress in our theoretical work of the one-dimensional, two-fluid plasma model in front of a negative electrode by adding the energy equation for ions into the equation set, which is an important step in modelling fusion-relevant plasmas. Even though the ions are born cold it was shown that they gain energy when approaching the limiting walls; however, they reach their maximum temperature before entering the plasma sheath. We also calculated the spatial profiles of the polytropic coefficient for ions. The maximum of the product of the polytropic coefficient profile and the ion temperature profile again marks the sheath edge. The agreement between the model and the kinetic particle-in-cell simulations is good.

In the field of **neutron transport calculations for fusion reactors** co-workers of the Reactor physics division have, in collaboration with colleagues from Culham Centre for Fusion Energy, United Kingdom, participated in preparations for the calibration of neutron detectors to 14-MeV neutrons. As part of these preparations we modelled a DT neutron generator and participated in the analysis of the responses to the various detectors in its surroundings. The DT generator was used as a calibration source for the calibration of the JET Tokamak in early 2017.

For the success of the calibration a good knowledge of the characteristics of the generator as a calibration source and the influence of the anisotropic source on the response of neutron detectors. The computational support in the characterization of the generator is crucial for the successful calibration of the detectors with a target uncertainty of 10%.

A parametric neutron source is used for the description of the plasma neutron source and we performed the analysis of the TT (tritium - tritium) plasma source, which will be used in the TT campaign of the JET Tokamak. The neutrons, originating from this reaction, are of particular interest, as three important reaction channels exist, through which neutrons with different energies are generated and the intensities of these channels are poorly known. Determination of the relative intensities of these three channels will be an important outcome of the TT campaign and the co-workers of F8 are engaged in computational support of the experiment. In 2016 we thus started the search for suitable detectors (mainly activation foils), to distinguish between the peaks in the TT reaction.

Co-workers of the F8 department have performed calculations of the neutron field inside the torus and along the tangential channel KM6\_T. It turned out that the flux and spectrum of the neutrons on the detectors in this channel are mainly due to direct neutrons of the plasma and from neutrons scattering from the collimator, and to a much smaller extent due to neutrons that are scattered through the remaining vacuum ports. This work is performed as part of the co-operation within the framework of the EUROfusion project within H2020.

In the framework of the European Fusion for Energy programme we collaborated in the following activities:

- Preparation and analysis of a benchmark experiment, which included the irradiation of a copper block (60 cm × 60 cm × 70 cm) with 14 MeV D-T neutrons. The aim was the validation of the neutron cross-sections of copper.
- Irradiation and analysis of Mn samples in the TRIGA reactor for the monitoring of tritium production.
- Evaluation and validation of the neutron cross-sections of iron.
- Validation of the photon data libraries on the basis of benchmark experiments from the SINBAD database.
- Analysis and validation of the DT neutron source modelling in the MCUNED code.

- In 2016 we commenced activities related to the ITER reactor, our task being the calculation of the effects of runaway electrons, specifically the production of gamma rays and their effect on the detection of gamma radiation originating from the plasma. The main part of the activities was aimed at the modification of the MCNP computational code to be able to perform calculations with an asymmetrical runaway neutron source using the existing ITER model. In the ITER project we are also involved in the computational support in the design of a neutron attenuator, which is required for the shielding of the detector of hard X rays.

**Organic semiconductors**, i.e., *organic light-emitting diodes, OLEDs* in displays of mobile devices and TV panels, *field-effect transistors, FETs*, photodiodes and organic photovoltaic cells, OPVCs, already represent nowadays the vital parts of various electronic devices that are available on the market. However, a wider use of these electronic elements is still effectively limited on account of the relatively slow transport of charges (holes as well as electrons) occurring within such materials. The stated shortcoming is evidenced, for instance, through the relatively weak current density in passive matrix displays and the switching time of FET transistors and due to the considerable difference in the velocity of electrons as compared to holes the reduction in the efficiency of the organic semiconductor light-emitting devices (recombination holes and electrons) as well as the resulting feeble electrical current from photovoltaic cells (due to the time delay in the arrival on the metal electrodes of each charge species arising from the electron-hole pairs).

However, it turns out (when considering a number of cases) that the current density diminishes with the increasing external electric field, which may be interpreted as an augmentation of the transparency for the charge transport within the organic semiconductor. On this basis it is conjectured that the increase of the relative degree of the crystalline order of the organic sample induces an enhancement of the effective charge mobility, resulting in the augmentation of the charge injection from the metal/organic interface into the organic bulk.

In the field of **medical physics** we continued the research focused on positron emission tomography (PET) image analysis, image-guided therapy of cancer, and modelling.

We performed a kinetic analysis study of dynamic FLT PET images, where sixteen canine cancer subjects were imaged dynamically with FLT PET/CT before and during radiotherapy. Kinetic analysis was assessed as a means to create multiple imaging biomarkers of resistance to radiotherapy from a dynamic FLT PET scan. A worse outcome after radiotherapy was associated with higher pre- or mid-therapy overall FLT  $K_r$ . Additionally, our data indicates that various imaging biomarkers derived from vascular parameters or their change through the therapy, contains even stronger prognostic information than the FLT transport parameter. The results will be published in a scientific journal.

We continued with the computational modelling of combined treatment with immunotherapy (programmed cell death 1 antibodies (anti-PD-1)) and radiotherapy. Preliminary results indicate that the expression of major histocompatibility complex I (MHC-I) on tumour cells might play an important role in tumour response to the aforementioned treatment. The model also predicts that hypofractionation should outperform stereotactic radiotherapy (SBRT) when combining radiotherapy with anti-PD-1. The results were presented at the AACR special conference *Tumour Immunology and Immunotherapy* in Boston, MA (20–23.10. 2016).

In collaboration with the Institute of Oncology Ljubljana we started a prospective study enrolling patients diagnosed with metastatic lung cancer after the failure of first- and second-line treatment, who will be treated with anti-PD-1 immunotherapy and imaged with diagnostic CT and FDG PET/CT. The aim of the study is to investigate whether radiomics analysis of FDG PET/CT scans better and more rapidly predicts the response to treatment with anti-PD-1 comparing with current standards (irRC).

Like all recent years, also in 2016 we had a close collaboration with the University of Wisconsin – Madison (USA).

## Some outstanding publications in the past year

1. Pregledni članek v ugledni reviji: Popov, Tsviatko K., Dimitrova, Miglena, Ivanova, Pavlina, Kovačič, Jernej, Gyergyek, Tomaž, Dejarnac, Renaud, Stöckel, Jan, Pedrosa, M. A., López-Bruna, D., Hidalgo, C. Advances in Langmuir probe diagnostics of the plasma potential and electron-energy distribution function in magnetized plasma. *Plasma sources science & technology*, ISSN 0963-0252, 2016, vol. 25, str. 1-18, ilustr. <http://iopscience.iop.org/article/10.1088/0963-0252/25/3/033001?fromSearchPage=true>, doi: 10.1088/0963-0252/25/3/033001.

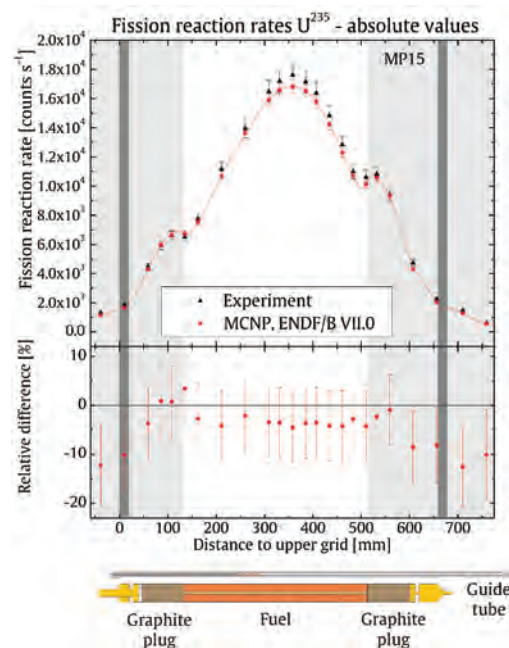


Figure 3: Comparison of measured and computed fission rate axial profiles in the core of the TRIGA reactor. The profiles were measured using miniature fission chambers. Schematics of the fuel element, fission chamber and instrumentation guide tube are shown in the bottom.

2. Gyergyek, Tomaž, Kovačič, Jernej. Ion temperature profiles in front of a negative planar electrode studied by a one-dimensional two-fluid model. *Physics of plasmas*, ISSN 1070-664X, Jun. 2016, vol. 23, no. 6, str. 1-18, ilustr. <http://dx.doi.org/10.1063/1.4953545>, doi: 10.1063/1.4953545.
3. Costea, Stefan, Fonda, Boris, Kovačič, Jernej, Gyergyek, Tomaž, Schneider, Bernd Sebastian, Schrittwieser, Roman, Ionița, Codrina. Bunker probe : a plasma potential probe almost insensitive to its orientation with the magnetic field. *Review of scientific instruments*, ISSN 0034-6748, 2016, vol. 87, no. 5, str. 1-4, ilustr. <http://scitation.aip.org/content/aip/journal/rsi/87/5/10.1063/1.4951688>, doi: 10.1063/1.4951688
4. M. Koželj, B. Cvikl, The negative mobility: An outcome of the electric field at the hole-injecting metal/organic semiconductor interface that varies as a linear function of the applied bias, *Thin Solid Films*, 616 (2016) 786-792.
5. Lengar, Igor, Čufar, Aljaž, Conroy, S., Batistoni, P., Popovichev, Sergei, Snoj, Luka, Syme, Brian, Vila, Rafael, Stankunas, Gediminas, et al, JET Contributors. Radiation damage and nuclear heating studies in selected functional materials during the JET DT campaign. *Fusion engineering and design*, ISSN 0920-3796. [Print ed.], 2016, vol. 109, str. 1011-1015, doi: /10.1016/j.fusengdes.2016.01.033.

### Awards and Appointments

1. Tanja Kaiba: Prešeren Award, Ljubljana, Slovenia, 6. 12. 2016, Faculty of Mathematics and Physics, University of Ljubljana, for the master thesis entitled: Fission and ionization chambers response at the JSI TRIGA reactor
2. Bor Kos: Young author award. Young author award committee at the international conference NENE 2016, Portorož, 5.-8. 9. 2016, for the contribution entitled "Variance Reduction of Fusion and Fission Neutron Transport Problems using the ADVANTG Hybrid Code" co-authored by Ivan A. Kodeli
3. Luka Snoj: Name of the Month on the Radio Val 202, June 2016, Ljubljana, Slovenia, awarded by RTV Slovenia, Radio Val 202

### Organization of Conferences, Congresses and Meetings

1. 25<sup>th</sup> International Conference "Nuclear Energy for New Europe" – NENE 2016, Portorož, Slovenia, 5.-8. 9. 2016
2. Student conference of the Reactor physics department (F-8) »Jožef Stefan« Institute, Ljubljana, Slovenia, 29. 2. 2016
3. 7FP GENTLE Intersemester Course »Nuclear Data Processing and Use in Nuclear Applications«, EC-JRC, Geel, Belgium, 14.-18. 11. 2016

### Patent granted

1. P. E. Galavis, Bhudatt R. Paliwal, James E. Holden, Robert Jeraj, System and method for gradient assisted non-connected automatic region (GANAR) analysis, US9355447 (B2), US Patent and Trademark Office, 31. 05. 2016

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## INTERNATIONAL PROJECTS

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. Development of Radiation Resistant Cameras<br/>Asst. Prof. Luka Snoj<br/>Isec Industrial Security Ab</li> <li>2. Overheating of Containers for Dry Storage of Spent Fuel after Full Blockage of Ventilation Channels<br/>Dr. Marjan Kromar<br/>Areva GmbH</li> <li>3. 7FP - CHANDA; solving CHallenges in Nuclear Data<br/>Prof. Ivan Aleksander Kodeli<br/>European Commission</li> <li>4. F4E-GRT-168.02; Specific Grant Agreement: Nuclear Data Improvements and Development of Tools - Nuclear Data Evaluation<br/>Prof. Ivan Aleksander Kodeli<br/>European Commission</li> <li>5. F4E-FPA-327 (PMS-DG): SG04; Conceptual Design and Interface Definitions for the Enabled ITER Radial Gamma-Ray Spectrometer Diagnostic<br/>Dr. Igor Lengar<br/>The European Joint Undertaking For The Development</li> <li>6. F4E-FPA-395-02; Gas Production Experiment and TBM Nuclear Instrumentation<br/>Prof. Ivan Aleksander Kodeli<br/>The European Joint Undertaking For The Development</li> </ol> | <ol style="list-style-type: none"> <li>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)<br/>Prof. Ivan Aleksander Kodeli<br/>IAEA - International Atomic Energy Agency</li> <li>8. Benchmarks of Computational Tools against Experimental Data on Fuel Burnup and Material Activation for Utilization, Operation and Safety Analysis of Research Reactors; Activation Rate Benchmark at the JSI TRIGA Mark-II Reactor<br/>Dr. Vladimir Radulović<br/>IAEA - International Atomic Energy Agency</li> <li>9. Training Costs for IAEA Fellowship for Mr. Mustafa Jaradat, JOR/14080; from 11 January 2016 to 10 March 2016<br/>Asst. Prof. Luka Snoj<br/>IAEA - International Atomic Energy Agency</li> <li>10. Training Costs for IAEA Fellowship for Mr. Mahmoud Mohamed, EGY/12023; from 1 August to 30 September 2016<br/>Asst. Prof. Luka Snoj<br/>IAEA - International Atomic Energy Agency</li> <li>11. E-SiCure - Engineering Silicon Carbide for Enhanced Border and Ports Security<br/>Asst. Prof. Luka Snoj<br/>Nato - North Atlantic Treaty Organisation</li> <li>12. H2020 - AIDA-2020; Advanced European Infrastructures for Detectors at Accelerators<br/>Dr. Vladimir Radulović<br/>European Commission</li> </ol> |
|---|---|

13. RU-FU, EUROFUSION; Research Unit - Administration and Services  
Asst. Prof. Luka Snoj  
European Commission
14. Exploitation of DT Operation for ITER-JET3-FU, EUROFUSION  
Asst. Prof. Luka Snoj  
European Commission
15. Education-ED-FU, EUROFUSION  
Asst. Prof. Luka Snoj  
European Commission
16. JET Enhancements-JET4-FU, EUROFUSION  
Dr. Igor Lengar  
European Commission
17. Impact of Neutron Irradiation in the Fusion Environment on Tritium Production, Tritium Retention and Nuclear Damage in Plasma Facing Materials  
Prof. Ivan Aleksander Kodeli  
Slovenian Research Agency
18. Experimental on-line neutron spectra adjustment method using various fission chambers with adequate fissile isotopes  
Dr. Gašper Žerovnik  
Slovenian Research Agency
19. Eksperimental validation of the gamma flux simulation scheme and measurement techniques by TLD, OSLD and ionization chamber in the mixed neutron-photon high dose rate environment of the JSI TRIGA reactor  
Asst. Prof. Luka Snoj  
Slovenian Research Agency
20. Mathematical methods for the nuclear data and code validation applied to improved safety of new nuclear reactor core design  
Prof. Ivan Aleksander Kodeli  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Reactor Physics  
Asst. Prof. Luka Snoj
2. Medical physics  
Prof. Robert Jeraj

## R & D GRANTS AND CONTRACTS

1. Development of methodology for calibration of neutron detectors with a 14.1 MeV neutron generator - JET fusion reactor case  
Asst. Prof. Luka Snoj
2. Analysis of material damage and activation in large scale fusion reactors - application to the reactor JET  
Dr. Igor Lengar

## 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  
Nuklearna Elektrarna Krško
2. Independent Evaluation of Modified Krško 16x16 VANTAGE+Fuel design fully in accordance with NEK Technical Specification SP-ES1250 Rev.0  
Dr. Marjan Kromar  
Nuklearna Elektrarna Krško d. o. o.

## VISITORS FROM ABROAD

1. Niklas Barringer, ISEC, Sweden, 12.-13. 1. 2016
2. Mustafa Jaradat, IAEA stipend, Jordan Atomic Energy Commission, Amman, Jordan, 11. 1.-10. 3. 2016
3. Stefan Costea, University Innsbruck, Innsbruck, Austria, 25. 4.-6. 5. 2016
4. Dr. Mitja Majerle, Nuclear Physics Institute, Rež, Czech Republic, 16. 5. 2016
5. Mahmoud Mohamed, IAEA stipend, Egyptian Nuclear and Radiological Regulatory Authority, Cairo, Egypt, 31. 7.-2. 10. 2016
6. Dr. Simon Pinches, scientific coordinator, ITER Organization, Confinement & Modelling Section, St Paul lez Durance, Cedex, France, 7.-8. 9. 2016
7. Prof. Gilles Bignan and dr. Christophe Destouches, CEA, Cadarache, France, 5. 9.-8. 9. 2016
8. Fausto Francescini, Westinghouse, Cranberry Township, Pennsylvania, USA, 5. 9.-8. 9. 2016
9. Prof. Helmuth Böck, TRIGA Reactor, Vienna, Austria, 5. 9.-8. 9. 2016
10. Stefan Costea, University Innsbruck, Innsbruck, Austria, 12. 9.-31. 10. 2016
11. Lars Öhlin, Head of Engineering Dept. and Jan Gunnarsson, ISEC, Helsingborg, Sweden, 13. 10. 2016
12. Prof. Tsviatko K. Popov, Faculty for Physics, University St. Kliment Ohridski, Sofia, Bulgaria, 20. 10.-30. 10. 2016
13. Shintaro Inoue, EUJEP2 student exchange, Tokyo Institute of Technology, School of Environment and Society, Transdisciplinary Science and Engineering - Nuclear Engineering, Tokio, Japan, 21. 11. 2016-18. 2. 2017
14. Mael Le Guillou and Adrien Gruel, CEA, Cadarache, France, 28. 11.-2. 12. 2016

## STAFF

### Researchers

1. Prof. Tomaž Gyergyek\*
2. Prof. Robert Jeraj
3. Prof. Ivan Aleksander Kodeli
4. Dr. Marjan Kromar
5. Dr. Igor Lengar
6. Asst. Prof. Luka Snoj, Head
7. Prof. Andrej Trkov
8. Dr. Gašper Žerovnik

### Postdoctoral associates

9. Dr. Jure Beričič, left 29.03.16
10. Dr. Dušan Čalič\*
11. Dr. Jernej Kovačič
12. Dr. Lucijan Plevnik, left 01.08.16
13. Dr. Vladimir Radulović
14. Dr. Urban Simončič

### Postgraduates

15. Klemen Ambrožič, B. Sc.
  16. Aljaž Čufar, B. Sc.
  17. Tanja Kaiba, B. Sc.
  18. Bor Kos, B. Sc.
  19. Vid Merljak, B. Sc.
  20. Žiga Štancar, B. Sc.
  21. Damijan Valentinuzzi, B. Sc.
- ### Technical and administrative staff
22. Slavko Slavič, B. Sc.
  23. Uršula Turšič, B. Sc.
  24. Bojan Žefran

Note:

\* part-time JSI member

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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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 the experimental techniques of particle physics to solve astrophysical problems. Slovenian researchers are participating in measurements of ultra-high-energy cosmic rays with the Pierre Auger observatory spread over a surface of 3000 km<sup>2</sup> near Malargue in Argentina.*



Head:  
**Prof. Marko Mikuž**

In order to reveal the ultimate secrets of nature in the world of elementary particles, accelerators with higher and higher energies are needed. Their cost, both in terms of money and human resources, has grown to the level where they are affordable only as joint international enterprises. Thus, future accelerators will be unique facilities 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 remain minute compared to that of the vast blast of the Big Bang that led to the creation of the Universe.

Together with colleagues from the Physics Department of the Faculty of Mathematics and Physics and the Faculty of Electrical Engineering of the University of Ljubljana, and from the Faculty of Chemistry and Chemical Technology of the University of Maribor, we are performing measurements at CERN and 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 2016 activities follows, focused on the contributions of our researchers:

## ATLAS experiment

In 2015 the upgraded Large Hadron Collider LHC began its operation at CERN and reached the record centre-of-mass energy of 13 TeV, which marks the beginning of the “Run 2” of LHC operation. In the following year 2016 the LHC then exceeded all expectations and facilitated the recording of the largest quantity of data at the ATLAS experiment so far. The amount of the ATLAS experiment proton-proton collision data at 13 TeV (Fig. 1) in 2016 is ten times larger than the data set collected in 2015, which led to the most precise Run 2 searches of new physics beyond the Standard Model achieved hitherto. In the analysed data a considerable number of different theories was excluded and there are some indications for potential new discoveries in the particle physics [1,2] – however, for confirming or refuting these a larger amount of data needs to be recorded and analysed. Subsequently, the next two years will be full of challenges and expectations of pivotal events. In 2016 the ATLAS collaboration published more than 100 scientific papers in the most distinguished scientific journals, bringing the total number of scientific papers published by the collaboration to 600, with more than a hundred additional papers in preparation.

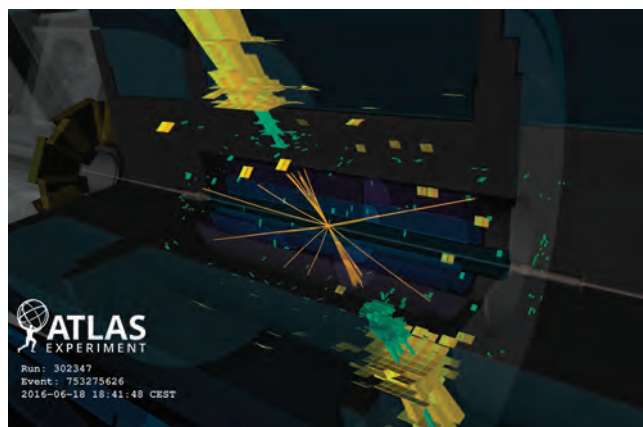


Figure 1: The event display of a proton-proton collision at the centre-of-mass energy of 13 TeV with the highest invariant mass of two jets in the resonance searches in the data collected in 2016 (Event 753275626, Run 302347). The two central jets have an invariant mass of 7.5 TeV.

**In 2016 the LHC exceeded all expectations and facilitated the recording of the largest quantity of data at the ATLAS experiment so far.**

The ATLAS Ljubljana group had a leading role in designing, building and operating several beam and radiation monitoring systems, namely: ATLAS Beam Condition Monitor (BCM), Beam Loss Monitor (BLM), Radiation Monitor (RADMON) and Diamond Beam Monitor (DBM). BCM was built to monitor conditions of the LHC beams and issue warnings at unexpected and potentially dangerous situations. In the first part of LHC operation it served

**Collaboration ATLAS intends to upgrade the detector in the next decade. The upgraded detector will be able to record the data even at the highest luminosity ( $5 \cdot 10^{34} \text{ cm}^2\text{s}^{-1}$ ) delivered by HL-LHC collider (High Luminosity LHC).**

as the main luminosity monitor of ATLAS. BLM on the other hand is solely a safety system and protected the ATLAS Inner Detector from potential damage by LHC beams which fired and extracted LHC beams a few times. RADMON records the doses received by different parts of the ATLAS Inner Detector. Newly built DBM was installed during the last shutdown and was used for the first time in 2015. Its readout is currently being developed. It is built from pCVD diamond sensor and pixel readout chip with pixels of size  $250 \times 50 \mu\text{m}^2$ . It will provide luminosity measurement complementary to the BCM and other luminosity monitors in ATLAS. It has prospects to become the main luminosity monitor with increasing luminosity when other detectors will start saturating.

Collaboration ATLAS intends to upgrade the detector in the next decade. The upgraded detector will be able to record the data even at the highest luminosity ( $5 \cdot 10^{34} \text{ cm}^2\text{s}^{-1}$ ) delivered by HL-LHC collider (High Luminosity LHC). The inner part of the detector will be replaced by a new tracker of charged particles with sensors based on semiconductor technology. Our department is involved in the development of sensors, readout electronics and support structures. The company ELGOLINE from Podskrajnik is fabricating multilayer flexible circuits, which will serve as the interface between the detector modules and the control electronics.

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

The data collected by the Belle detector at the electron-positron collider KEKB in Tsukuba, Japan, are being exploited by members of the department to carry out precise measurements of rare processes in the world of subatomic particles. By comparing the results of measurements and theoretical predictions it is possible to check for possible contributions from New Physics, the yet unknown particles and processes. These processes are - among others - also responsible for the fact that we live in a universe in which matter (particles) completely dominates over antimatter (antiparticles). The measurements performed by the Belle and Belle II collaborations are part of the so-called intensity frontier that complements research efforts in the Cosmic and Energy Frontiers. The measurements performed using the collision data collected by the Atlas experiment at the LHC in CERN falls into the latter group.

**A large fraction of the activity of the Ljubljana Belle team was devoted to the preparation of the follow-up Belle II experiment.**

In 2016, the most interesting results published by the researchers of the international research group Belle (542 researchers from 89 institutions and 20 countries) were measurements of branching fractions of the decays  $B \rightarrow D^{(*)} \tau \mu$  and measurement of tau lepton polarisation in these decays and full angular analysis of  $B \rightarrow K^* l l$  decays, where  $l$  represents light lepton: electron or muon [3].

Both types of decays probe lepton flavour universality, which is one of the most profound properties of the Standard Model of interactions between the fundamental particles. Lepton flavour universality states that the coupling of the leptons to gauge bosons are flavour-independent (i.e., the interactions between leptons and gauge bosons are the same for all leptons). Using above decays we can test whether the couplings to leptons in nature are really flavour-independent. The results of the measurements indicate that the couplings are not flavour-independent and that the lepton flavour universality is violated, however the significance of the violation is not high enough. The much larger data sample that will be collected by the Belle II experiment will allow for more precise tests and a confirmation of the current deviation, which would represent an unambiguous proof of New Physics (Fig. 2).

In the past year we have performed as well a study of radiative charm decays, which resulted in the first observation of the  $D_0 \rightarrow \rho \gamma$  decays, first measurement of CP violation in radiative charm decays [4] and improved measurement of branching fractions of  $D_0 \rightarrow \Phi \gamma$  and  $K(892)^* \rightarrow \gamma$  decays. Measurements will enable tests of long-distance dynamics calculations on the lattice that dominate in these decays. Measurements of CP violation in radiative decays are sensitive to the contributions of non-standard chromomagnetic dipole operators and complementary to the existing measurements performed using hadronic or (semi-)leptonic decays. The results are consistent with the Standard Model predictions with uncertainties. More stringent tests will be performed using the data collected by the Belle II experiment.

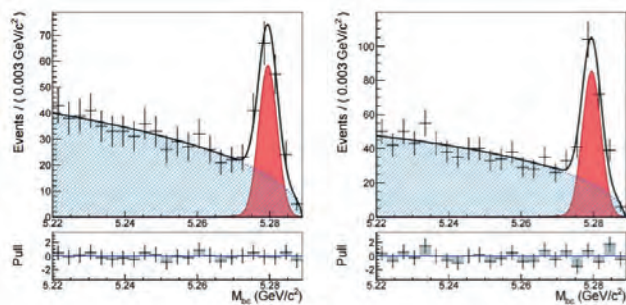


Figure 2: Signal of  $B \rightarrow K^* e^+ e^-$  (left) and  $B \rightarrow K^* \mu^+ \mu^-$  (right) decays [3]. Possible difference in the heights of the two signal peaks would be a sign of lepton universality violation.

A large fraction of the activity of the Ljubljana Belle team was devoted to the preparation of the follow-up Belle II experiment. Belle II is again an international collaboration with more than 700 scientists from 96 institutions and 23 countries. In 2016, the group reached several important milestones. The central drift chamber was successfully installed in the Belle II spectrometer.

In 2016 we have also successfully completed the assembly of one of the most delicate parts of the detector, the TOP (Time-Of-Propagation) counter (Fig. 3). This detector component is intended for the identification of charged particles through the detection of Cherenkov light; this light is emitted by very fast particles in a 2-cm-thick quartz plate. All 16 modules were installed in the spectrometer, and are currently being tested with cosmic rays. In the meantime, we have also started the assembly of the detector to identify particles in the forward region, the ARICH (Aerogel Ring Imaging Cherenkov)

counter, our main responsibility in the Belle II detector preparation. We note that one of the key components, the low noise read-out electronics printed circuit boards for the ARICH counter were manufactured in Slovenia.



Figure 3: Placement of quartz radiators for Time-Of-Propagation counter

### Pierre Auger observatory

The Pierre Auger Observatory is an international cosmic-ray observatory in Argentina designed to detect ultra-high-energy cosmic rays: sub-atomic particles traveling nearly at the speed of light and each with energies beyond  $10^{18}$  eV. In Earth's atmosphere such particles interact with air nuclei and produce various other particles. Secondary particles forming the so-called "air shower" can be detected and measured in order to clarify the origin of the highest-energy primary particles and their properties like energy, arrival direction and the particle type (photons, protons, atomic nuclei). But since these high-energy particles have an estimated arrival rate of just 1 per  $\text{km}^2$  per century, the Auger Observatory has created a detection area of  $3000 \text{ km}^2$  to be able to record a large number of these events. It is located in the western Mendoza Province, Argentina, near the Andes.

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 Collaboration had shown that the energy spectrum of cosmic rays exhibits a sharp drop around  $10^{20}$  eV. This drop is compatible with the Greisen-ZatsepinKuz'min (GZK) cut-off caused by the universe becoming opaque due to resonant collisions between ultra-high-energy protons and the photons of the cosmic microwave 2.7-K background radiation. Past measurements by the Pierre Auger Collaboration already have cast some doubt on this explanation, and this year's results further established that the GZK cut-off cannot be the entire story and even the extent of its contribution to the cut-off remains unclear.

Collisions of ultra-high-energy cosmic rays with atmospheric molecules provide hadronic interactions at an energy that exceeds the LHC centre-of-mass energy by one-to-two orders of magnitude. Although progress was made in incorporating LHC results, some mysteries were not solved. The number of muons in Monte Carlo simulations is very significantly smaller than the number measured in experimental data. Also the depth at which most muons are produced that reach the Earth's surface cannot be described by Monte Carlo simulation for any reasonable composition mix of cosmic rays.

The weak anisotropy signal that remains in the Auger data is affected by cosmic ray masses and charges. Auger data indicate that the most energetic particles are not only protons but mostly heavy, highly-charged, nuclei. These are deflected by cosmic magnetic fields, which makes it difficult to track back to their origin.

To address this challenge the Pierre Auger observatory is currently upgrading its detection capabilities. The key element of the upgrade will be the installation of a plastic scintillator on top of each existing surface detector station. It will provide a complementary measurement of the showers allowing the reconstruction of muons and electromagnetic particles. The surface scintillator detector stations (SSD) will be deployed over the full  $3,000\text{-km}^2$  area of the overall surface detector (SD). To enhance the capabilities of the surface detector, especially for composition measurements, it will be equipped with upgraded electronics with a larger sampling rate and a larger dynamic range.

### Distributed computing

The SiNET Tier-2 distributed computing centre with a computing power of 5200 cores and storage capacity of 4000TB continued to provide resources to ATLAS, Belle II and Pierre Auger experiments. The local storage sys-

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**The Pierre Auger Collaboration had shown that the energy spectrum of cosmic rays exhibits a sharp drop around  $10^{20}$  eV.**

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tem was upgraded with CephFS technology, which delivers much higher throughput and faster data access than the previous NFS-based solution, reaching data-processing rates up to 200TB per day. An automatic execution of payloads within Linux containers has been deployed using Singularity and Docker. This will enable customized operating-system environments to the experiments. Existing LHCONE network bandwidth was frequently reaching the bandwidth saturation in 2016 due to unexpectedly successful LHC operation delivering 50% more data than initially expected, so preparations for the upgrade to 20 Gb/s bandwidth were initiated end of 2016.

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 Jožef Stefan Institute, Arnes, Actur, 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 international organizations EGI/InSPIRE, wLCG and Nordugrid and had participated in several joint projects related to the support, maintenance and planning of the computing infrastructure as well as the development, distribution and deployment of the distributed computing infrastructure.

### Detector development

We continued the research of particle detectors developed in HV-CMOS technology, which enables cost effective and large series production of sensors. The HV processes allow the connection of a substrate to high voltage, which makes the charge drift the dominant component contributing to the signal. The ability to integrate first amplification and further processing stages in the sensor allows for excellent signal-to-noise ratio and very efficient operation. In 2016 we measured the charge-collection properties of many detectors after irradiations with reactor neutrons and 24-GeV protons. We have systematically determined the changes of space-charge concentration with a fluence

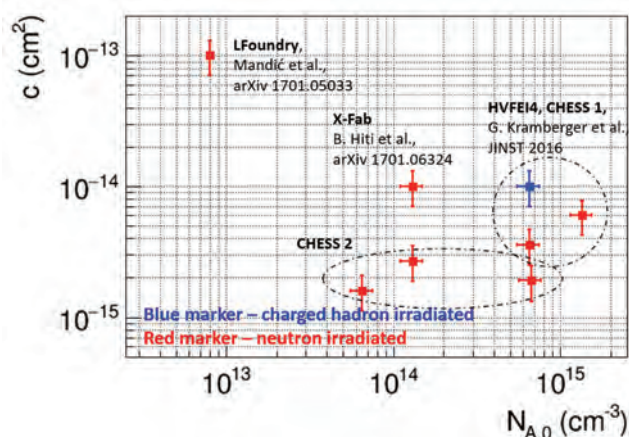


Figure 4: Variation of space charge concentration with fluence for detectors with different substrate resistivities.

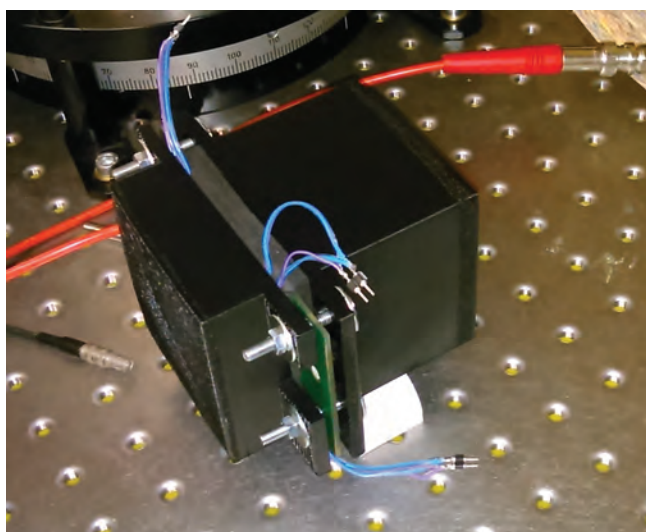


Figure 5: A prototype of annihilation gamma photon detector with improved spatial resolution, based on LYSO crystal matrix segmented to cells with sides of 1.5 mm.

for detectors with different substrate resistivities (Fig 4). The measurements included almost all prototype detectors for application at the upgraded LHC.

In the past year we joined the project that aims at building a High Granularity Timing Detector for ATLAS. We took the leading role in radiation studies of Low Gain Avalanche Detectors (LGAD), which are the baseline choice for the sensor technology. We have determined the dependence of gain on fluence and voltage and showed that for thin LGAD detectors the decrease of gain with voltage can be compensated by higher applied voltage for almost the entire range of expected fluences at HL-LHC. A single sensor (50  $\mu\text{m}$ ) time resolutions of 26 ps was achieved before irradiation.

Explorations of diamond detectors lead to first measurements of charge multiplication in diamond particle detectors. We showed that electric fields of 100 V/ $\mu\text{m}$  were required and could be achieved by special electrode configuration.

A multichannel system for simultaneous readout of different dosimetric sensors was intensively tested. Apart from its use in medical applications the system is used also for precise dosimetric measurement during irradiations at the JSI reactor facility.

We continued with the development of new methods for the detection of annihilation gamma rays in positron emission tomography (PET), one of the most important medical imaging methods. We have already shown that the difference in the time of flight of the two gamma rays can be measured with a very high precision of 80ps (FWHM) if a Cherenkov radiator is used as a gamma-ray converter instead of a scintillator. With such a resolution, we can directly obtain a three-dimensional information on the emission point of the two gamma rays, which substantially reduces the time needed to determine the activity distribution in the patient. While this first result was achieved with a microchannel plate photomultiplier tube (MCP PMT) as the low level light sensor, we have in 2016 continued with the examination of possibilities offered by silicon photomultipliers (SiPM), compact semiconductor based light sensors that can be operated in high magnetic fields (important for multimodal imaging in combination with MRI), and would be much cheaper. The results have shown that by using single Cherenkov photon hits, a resolution can be achieved that is better than 200 ps. We have also started to investigate how the resolution could be improved in multi-hit cases.

Within the frame of research of particle physics detectors in medical physics we have performed characterization of low-gain avalanche diodes (LGAD) matrices. The measurements will be used in element selection for suitability study of a Compton camera with LGAD detectors for proton therapy.

We developed a prototype of annihilation gamma photon detector with improved spatial resolution, based on LYSO crystal matrix segmented to cells with sides of 1.5 mm. The prototype is shown in the attached photograph (Fig. 5). Tasks related to LYSO prototype development and evaluation were also performed.

Within the CIMA international collaboration consisting of scientists from Ohio State University (OSU), University of Michigan (UM), University of Valencia and JSI we have continued to evaluate the prototype of a high-resolution PET system with silicon detectors at OSU. We have continued the analysis of recorded images.

Within the framework of the European project AIDA 2020 (Advanced European Infrastructures for Detectors at Accelerators) more than 180 irradiations by neutrons were performed at the reactor centre at the request of 22 different institutions. The focus was on the development of components for planned upgrades of ATLAS, CMS and Belle detectors.

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**Explorations of diamond detectors led to the first measurements of charge multiplication in diamond particle detectors.**

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## Organization of Conferences, Congresses and Meetings

1. The 9th International Workshop on Ring Imaging Cherenkov Detectors (RICH 2016), Bled, Slovenia, 5 - 9 September 2016
2. 2nd TCT Workshop 2016, Jožef Stefan Institute, Ljubljana, Slovenia, 17 - 18 October 2016

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## INTERNATIONAL PROJECTS

1. COST TD1401; Fast Advanced Scintillator Timing (FAST)  
Prof. Peter Kriz̃an  
Cost Office
2. COST CA16108 - VBSCan; Vector Boson Scattering Coordination and Action Framework  
Prof. Borut Paul Kerševan  
Cost Office
3. H2020 - JENNIFER; Japan and Europe Network for Neutrino and Intensity Frontier  
Experimental Research  
Prof. Peter Kriz̃an  
European Commission
4. H2020 - AIDA-2020; Advanced European Infrastructures for Detectors at Accelerators  
Prof. Marko Mikuž  
European Commission
5. Measurement of Rare Semileptonic B Meson Decays and Construction of Belle II Detector  
Asst. Prof. Anže Zupanc  
Slovenian Research Agency
6. Development of New Detectors for Medical Imaging  
Prof. Marko Mikuž  
Slovenian Research Agency
7. Development of Silicon and Diamond Semiconductor Detectors for Particle Physics Experiments and Medical Imaging  
Prof. Vladimir Cindro  
Slovenian Research Agency
8. Studies of Silicon Detector Properties by Using Transient Current Technique  
Dr. Gregor Kramberger  
Slovenian Research Agency

## RESEARCH PROGRAMS

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

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## R & D GRANTS AND CONTRACTS

1. ATLAS Diamond Beam Monitor  
Prof. Marko Mikuž
2. Search for microscopic black hole signatures with ultra-high energy cosmic rays  
Prof. Marko Zavrtanik
3. Novel scintillation detectors for precision particle physics experiments  
Prof. Peter Kriz̃an
4. History of Doctoral Dissertations by Slovene Candidates in the Austro Hungarian Empire (1872/1918)  
Prof. Boštjan Golob
5. Novel detection methods based on Cherenkov radiation  
Prof. Peter Kriz̃an
6. Development of in-vivo dosimetry for applications in radiotherapy  
Dr. Gregor Kramberger
7. Collaboration CERN RD-39  
Prof. Marko Mikuž  
Cern
8. Collaboration CERN RD-50  
Prof. Marko Mikuž  
Cern
9. Collaboration DELPHI  
Prof. Borut Paul Kerševan  
Cern
10. Collaboration ATLAS  
Prof. Marko Mikuž  
Cern
11. Collaboration CERN RD-42  
Prof. Marko Mikuž  
Cern
12. Collaborations Belle in Belle II  
Prof. Peter Kriz̃an  
Kek - High Energy Accelerator Research
13. Design, Procurement and QA of Flex-rigid Hybrids  
Prof. Marko Mikuž  
European Organization For Nuclear Research
14. Conference „RICH 2016“ - The 9th International Workshop on Ring Imaging Cherenkov Detectors; Bled, Slovenia, 5.-9.9.2016  
Prof. Peter Kriz̃an

## VISITORS FROM ABROAD

1. Kazuho Kobayashi, University of Nagoya, Nagoya, Japan, 30. 5. - 15. 7. 2016
2. Mosee Mariotti, INFN - Istituto Nazionale di Fisica Nucleare, Padova, Italy, 19. 5. - 20. 5. 2016
3. Riccard Rand, INFN - Istituto Nazionale di Fisica Nucleare, Padova, Italy, 19. 5. - 20. 5. 2016
4. Marko Milovanović, Deutsches Elektronen-Synchrotron (DESY), Zeuthen, Germany, 20. 6. - 24. 6. 2016
5. Emanuell Callvaro, IFAE - Institute for High Energy Physics, Barcelona, Spain, 13. 6. - 24. 6. 2016
6. Maizura Binti Ibrahim, Waste Technology Development Center (Malaysian Nuclear Agency), Malaysia, 14. 8. - 30. 9. 2016
7. Mario del Mar Carulla iz "Centro Nacional de Microelectrónica (IMB-CNM-CSIC), Univ. Autónoma de Barcelona", Barcelona, Spain, 21. 8. - 13. 9. 2016
8. Sachi Tamechika, Tokyo Metropolitan University, Tokyo, Japan, 30. 9. - 2. 11. 2016
9. Emanuell Callvaro, IFAE - Institute for High Energy Physics, Barcelona, Spain, 16. 10. - 20. 10. 2016
10. Dania Consuegra Rodriguez, master of physics, University of Santa Cruz, Bahia, Brazil, 3. 11. - 31. 12. 2016
11. Marko Milovanović, Deutsches Elektronen-Synchrotron (DESY), Zeuthen, Germany, 16. - 19. 11. 2016
12. Nataša Savić, Max Planck Institut für Physik, Munich, Germany, 11. 12. - 15. 12. 2016

## STAFF

### Researchers

1. Asst. Prof. Marko Bračko\*
2. Prof. Vladimir Cindro
3. Prof. Andrej Filipčič
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. Dr. Boštjan Maček
11. Asst. Prof. Igor Mandić
12. Prof. Marko Mikuž\*, Head
13. Dr. Rok Pestotnik
14. Asst. Prof. Tomaž Podobnik\*
15. Prof. Marko Starič
16. Prof. Marko Zavrtanik
17. Prof. Danilo Zavrtanik\*
18. Asst. Prof. Anže Zupanc
19. Asst. Prof. Dejan Žontar\*

### Postdoctoral associates

20. Dr. Jyoti Prakash Biswal, left 01.11.16

21. Dr. Andrej Studen

### Postgraduates

22. Bojan Hitl, B. Sc.
23. Luka Kanjir, B. Sc.
24. Matic Lubej, B. Sc.
25. Manca Mrvar, B. Sc.
26. Miha Muškinja, B. Sc.
27. Tara Nanut, B. Sc.
28. Tadej Novak, B. Sc.
29. Grygorii Sokhrannyi, B. Sc.
30. Tina Šfiligoj, B. Sc.
31. Dr. Elvedin Tahirović, left 01.02.16

### Technical and administrative staff

32. Andreja Butina
33. Jurij Eržen
34. Dejan Lesjak
35. Erik Margan

Note:

\* part-time JSI member

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## PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

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## PUBLISHED CONFERENCE CONTRIBUTION

1. M. Artuso *et al.* (128 authors), "A 3D diamond detector for particle tracking", In: *Frontier Detectors for Frontier Physics: Proceedings of the 13th Pisa Meeting on Advanced Detectors*, La Biodola, Isola d'Elba, May 24-30, 2015, *Nucl. Instrum., Methods Phys. Res., Sect. A, Accel.*, vol. 824, pp. 402-405, 2016.
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8. Z. Liang *et al.* (58 authors), "Study of built-in amplifier performance on HV-CMOS sensor for the ATLAS phase-II strip tracker upgrade", In: *Proceedings of the 10th International "Hiroshima" Symposium on the Development and Application of Semiconductor Tracking Detectors*, Xi'an, China, 25-29 September 2015, *Nucl. Instrum., Methods Phys. Res., Sect. A, Accel.*, vol. 831, pp. 156-160, 2016.
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## MENTORING

1. Jyoti Prakash Biswal, *Measurement of  $c\bar{c}c$  production in  $e^+e^-$  annihilation*: doctoral dissertation, Ljubljana, 2016 (mentor Marko Bračko).
2. Elvedin Tahirovič, *Aerogel ring imaging Cherenkov detector with silicon photomultipliers*: doctoral dissertation, Ljubljana, 2016 (mentor Rok Pestotnik).
3. Barbara Krašovec, *Distributed computing as a service with ARC middleware*: master's thesis, Ljubljana, 2016 (mentor Mojca Cigliarič; co-mentor Andrej Filipič).
4. Miha Kovačič, *Retrospective analysis of the frequency and severity of radiation-induced skin injuries from interventional radiology procedures*: master's thesis, Ljubljana, 2016 (mentor Dejan Žontar; co-mentor Nejc Mekiš).
5. Martin Lozar, *Sistem za verzioniranje dokumentov*: master's thesis, Nova Gorica, 2016 (mentor Andrej Filipič).
6. Anže Medved, *Karakterizacija čitalne elektronike za detektor obročev Čerenkova pri Belle II*: master's thesis, Ljubljana, 2016 (mentor Rok Pestotnik).
7. Tadej Novak, *Zaznavanje nabitih delcev s pasovnimi silicijevimi detektorji pri preletu pod velikimi koti*: master's thesis, Ljubljana, 2016 (mentor Marko Mikuž; co-mentor Gregor Kramberger).
8. Nina Verdel, *Silicijeva fotopomnoževalka kot senzor svetlobe Čerenkova pri pozitronski tomografiji*: master's thesis, Ljubljana, 2016 (mentor Peter Križan; co-mentor Rok Dolenc).

# 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**

The structural chemistry of inorganic fluorides is dominated by the simple electrostatic and geometrical principles for which the coordination number of six with an octahedral coordination is favoured for nearly all transition metals. Instead of being isolated, the resulting octahedra can share their F ligands, forming oligomeric or polymeric species. The crystal-structure determination of  $[\text{XeF}_5]_5[\text{Ti}_{10}\text{F}_{45}]^-$  reveals the largest known oligomeric fluoro-metallate  $[\text{Ti}_{10}\text{F}_{45}]^-$  anion built from ten  $\text{TiF}_6$  octahedra, sharing vertices, in the shape of a double-star. The study of the  $\text{XeF}_6/\text{TiF}_4$  system has been reported by Z. Mazej and E. Goresnik (JSI) in New J. Chem. The contribution was selected for the inside-front cover of the September issue. Additional studies were also made with group-12 metal cations and the  $\text{TaF}_5$  Lewis acid. Reactions in a 1:2 ratio yielded  $\text{M}(\text{TaF}_6)_2$  compounds, while excess of  $\text{TaF}_5$  led to the formation of undecafluoridoditantalate anions connecting metal cations into a 1D structure.

Within the research of nanostructured metal fluorides, the course of solvothermal processes under different temperature regimes was followed on a modified device for the preparation of these materials. The established methodology provides a better insight into the development of the morphology of the primary fluoride nanoparticles during processing, which is the basis for the further development and optimization of these synthetic procedures.

In the research of solid acids based on  $\text{H}_3(\text{P}(\text{W}_3\text{O}_{10})_4)$ , a series of solid products was prepared by a partial or complete replacement of  $\text{H}^+$  in the original heteropolyacid with some metal cations (eg.  $\text{Zn}^{2+}$ ,  $\text{Al}^{3+}$  or  $\text{Ga}^{3+}$ ), and their acidity was studied. These materials can serve as perspective (super)acidic catalysts for the technically interesting conversion of methane into higher hydrocarbons. This research is conducted in collaboration with the National Institute of Chemistry.

In cooperation with the K5 and K9 departments and other research institutions, we have studied domain-wall conduction in ferroelectric  $\text{BiFeO}_3$  controlled by the accumulation of charged defects and published the results in Nature Materials.

The search for a nucleophilic fluorinating agent in an organic solvent led to reactions of N-heterocyclic carbene (1,3-Bis(2,6-diisopropylphenyl)-1,3-dihydro-2H-imidazol-2-ylidene;  $\text{L}^{\text{Dipp}}$ ) with different sources of hydrofluoric acid ( $\text{Et}_3\text{N}\cdot 3\text{HF}$ , anhydrous hydrogen fluoride and  $\text{KHF}_2$ ) in 1:1, 1:2, 1:3 ratios. Isolated salts  $[(\text{L}^{\text{Dipp}})\text{H}]^+[\text{F}]^-$ ,  $[(\text{L}^{\text{Dipp}})\text{H}]^+[(\text{HF})\text{F}]^-$  and  $[(\text{L}^{\text{Dipp}})\text{H}]^+[(\text{HF})_2\text{F}]^-$  show such possibilities.  $[(\text{L}^{\text{Dipp}})\text{H}]^+[\text{F}]^-$ , which shows the characteristics of a free fluoride reagent, can be obtained with a good yield and without the contaminants usually present in such compounds.

In 2016 the direct synthesis of copper compounds was performed. Dissolving elemental copper in a  $\text{CBr}_4$ -DMSO mixture in the presence of hexamethylenetetramine (*hex*) resulted in the formation of  $\text{CuBr}(\text{hex})_2$  and  $\text{Cu}(\text{DMSO})_6\cdot\text{Cu}_2\text{Br}_6$  compounds. Using *dabco* (1,4-diaza-bicyclo [2.2.2] octane) instead of *hex*  $[\text{Cu}^{\text{I}}(\mu\text{-Br})_2(\text{H}^+\text{dabco})\text{Cu}^{\text{I}}(\mu\text{-Br})(\kappa\text{-S-DMSO})_n]$  compound was obtained. The comproportionation reaction of  $\text{CuCl}_2\cdot 2\text{H}_2\text{O}$  and copper powder in the presence of *dabco* in DMSO results in the formation of the  $\text{Cu}_3\text{Cl}_3(\text{dabco})(\text{DMSO})$  complex. All the mentioned complexes were characterized by the X-ray single-crystal technique and by Raman spectroscopy.

The new composite materials ( $\text{MoS}_2/\text{C}$ ) containing  $\text{MoS}_2$  particles embedded in a carbon matrix were synthesized in a single-step process by sulphidation of the  $\text{MoO}_2(\text{AcAc})_2$  ( $\text{AcAc}$  = acetylacetonato) coordination compound. The

## New fluorinating reagent, based on the N-heterocyclic carbene, was synthesized.

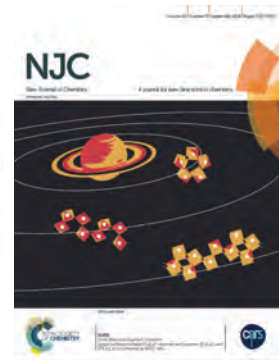
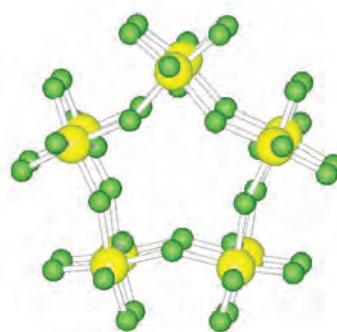


Figure 1: a.) the largest known discrete decameric  $[\text{Ti}_{10}\text{F}_{45}]^{5-}$  anion built from ten  $\text{TiF}_6$  octahedra, sharing vertices, in the shape of a double-star. b.) Inside cover of the New Journal of Chemistry issue 9, 2016 (cover designed by M. Mazej)

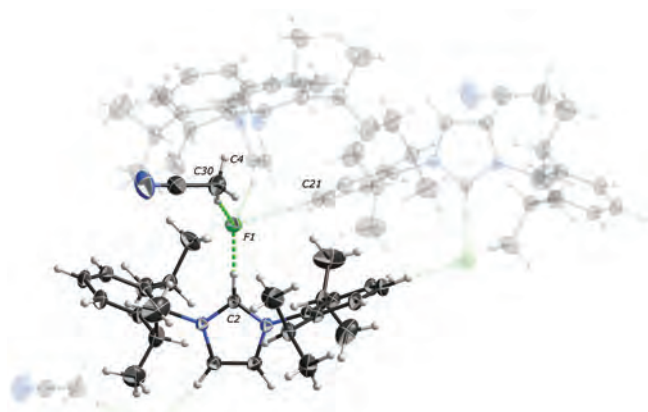


Figure 2: Structure of the [(LDipp)H]<sup>+</sup>[F]<sup>-</sup>

**Technical leadership of the international consortium for the large audit of the process safety management system at a client from the oil and gas industry outside Slovenia.**

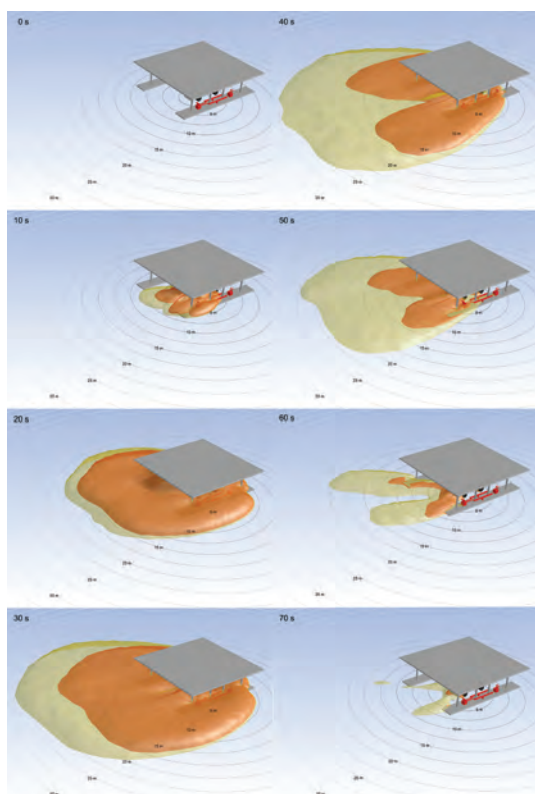


Figure 3: Results from the CFD simulation of propane jet release, impingement and dispersion under the roof - cloud shape animation based on time. Orange and yellow colours represent LFL and LFL/2 propane concentrations in the air, respectively.

lower temperature MoS<sub>2</sub>/C composites exhibit a higher activity compared to the commercial MoS<sub>2</sub> powder in hydrodeoxygenation reactions.

The composition dependence of radio-frequency plasma polymerized toluene on a composition of starting plasma gases toluene and ammonia was studied by vibrational spectroscopy and contact-angle measurements. The plasma-polymerized surfaces where the ammonia concentration in the plasma gas varied between 10 % to 50 % exhibit very similar surface properties, which was revealed by the contact angles appearing in the range from 95.4 to 98.9 degrees.

Within the topic of the process safety, we concluded the EU 7th FP project TOSCA (Total Operations Management for Safety Critical Activities) in which we participated as a partner. The project was dealing with the integration of the individual management aspects industrial operations as a total safety, quality and productivity management system (at the company level). In this year we concluded the reporting about the implementation, testing and evaluation of the efficiency of TOSCA products (methods and tools) in 12 case studies, where we contributed as a lead author in four papers in recognized scientific journals. Partners, industrial stakeholders and reviewers positively evaluated the proposed project solutions, tools and methods, for example, related to the management of safety-relevant changes in organizations, planning of rare potentially hazardous work procedures, as well as modelling of hazardous material releases in complex conditions.

In this year we took a technical lead of an international consortium for consultation project for industrial client outside Slovenia. More specifically, it was about the initial audit of the process safety management system within the rather large organization in the oil and gas industry. The work done was the basis for setting the priorities for the safety management system improvements in 2017 and beyond.

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 and ended this year. In the project, which dealt with the assessment and preparedness for terrorist risks (aspect of security), we participated on the basis of our previous experiences in the assessment of such threats to industrial operations.

A supermonitoring of guarantee measurements of the Flue Gas Desulphurization Plant of unit 6 in the Šoštanj Thermal Power Plant in collaboration with partners was conducted. In collaboration with the Materials Synthesis department the dissolution mechanism of upconverting AYF<sub>4</sub>:Yb,Tm (A = Na or K) nanoparticles in aqueous media was suggested. Degradation of NaYF<sub>4</sub>:Yb,Tm-based upconversion nanoparticles in phosphate buffered saline solution was studied and the luminescence lifetime of the 800-nm upconversion emission was identified as an optimum parameter for stability screening of and monitoring of changes in particle surface chemistry. We continued with writing review articles for Structural Chemistry journal; to a short summary of each article, a thermochemical comment and suggestions for future research are added.

The activity in the field of education and the promotion of sciences should be mentioned. Members of the department were actively engaged in the work of the Jožef Stefan International Postgraduate School as lecturers and as mentors to M.Sc. and Ph.D. students. In addition, the School of Experimental Chemistry maintained its very important relations with elementary, secondary schools and even kindergartens through experimental courses performed in a specialised laboratory or through direct demonstrations at the schools. With demonstrations of chemical experiments, we participated at the 22th Slovenian Science Festival, organized by the Slovenian Science Foundation and at the Hokus pokus and Lupa festival. Some of the activities of the School of the 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 year

- Zoran Mazej, Evgeny A. Goreschnik, Largest perfluorometallate [Ti<sub>10</sub>F<sub>45</sub>]<sup>5-</sup> oligomer and polymeric ([Ti<sub>3</sub>F<sub>13</sub>]<sup>-</sup>)<sub>∞</sub> and ([TiF<sub>5</sub>]<sup>-</sup>)<sub>∞</sub> anions prepared as [XeF<sub>5</sub>]<sup>+</sup> salts, *New J. Chem.* 40, (2016) 7320-7325.

2. Tadej Rojac, Andreja Benčan, Goran Dražič, Naonori Sakamoto, Hana Uršič, Boštjan Jančar, Gašper Tavčar, Maja Makarovič, Julian Walker, Barbara Malič, Dragan Damjanović, Domain-wall conduction in ferroelectric BiFeO<sub>3</sub> controlled by accumulation of charged defects", *Nature materials*, (2016) 7, [in press]
3. Dominik Kurzydłowski, Tomasz Jaroń, Andrzej Ozarowski, Stephen Hill, Zvonko Jagličič, Yaroslav Filinchuk, Zoran Mazej, Wojciech Grochala, Local and cooperative Jahn-Teller effect and resultant magnetic properties of M<sub>2</sub>AgF<sub>4</sub> (M = Na-Cs) phases, *Inorg. Chem.*, 55 (2016) 11479-11489.
4. Blaž Alič, Gašper Tavčar, "Reaction of N-heterocyclic carbene (NHC) with different HF sources and ratios: a free fluoride reagent based on imidazolium fluoride", *J. Fluorine Chem.*, 192 (2016) 141-146.
5. Marko Gerbec, "Safety change management - a new method for integrated management of organizational and technical changes", *Saf. sci.*, (2016) 10 [in press]
6. Matic Lozinšek, Gary J. Schrobilgen, "The world of krypton revisited", *Nature Chem. (Print)*, 8 (2016) 732.

## Patent granted

1. Andrej Kovič, Adolf Jesih, Aleš Mrzel, Process for the synthesis of the molybdenum carbide in the form of quasi-one-dimensional structures, that is, nano-wires, micro-wires, nano-strips and micro-strips, SI24925 (A), Slovenian Intellectual Property Office, 31. 08. 2016.

## INTERNATIONAL PROJECTS

1. Export of the Fluorinated Carbons  
Dr. Zoran Mazej
2. Extraction of Tantalum and Niobium from Ores  
Asst. Prof. Gašper Tavčar  
Prg Ltd.
3. 7FP - TOSCA; Total Operations Management for Safety Critical Activities  
Asst. Prof. Marko Gerbec  
European Commission
4. 7FP - FluoCoorChem; Fluorinated Weakly Coordinating Anions for Coordination Chemistry of Unusual Ligands  
Dr. Matic Lozinšek  
European Commission

## R & D GRANTS AND CONTRACTS

1. Direct Conversion of Methane to Higher Hydrocarbons Using Superacid Catalysts  
Asst. Prof. Gašper Tavčar
2. Implementation of Process Safety Management System (PSMS) into NIS j.s.c.  
Asst. Prof. Marko Gerbec  
European Virtual Institute For Integrated Risk

## NEW CONTRACT

1. A supermonitoring of the guarantee measurements of the Flue Gas Desulphurization Plant of unit 6 of the Šoštanj Thermal Power Plant  
Prof. Maja Ponikvar-svet  
Teš d. o. o.

## RESEARCH PROGRAM

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

## VISITORS FROM ABROAD

1. Prof. dr. Wojciech Grochala, Working visit, University of Warsaw, Warsaw, Poland, 7.10. - 11.10. 2016
2. Kristiina Penttila, Sanna Holappa, Working visit, Raahen ammattiopisto, Raahen, Finland, 7.6. - 9.6. 2016
3. Estela Herbst, Student exchange, Universidade Federal de São Paulo, São Paulo, Brazil, 10.8. - 10.10. 2016

## STAFF

### Researchers

1. Asst. Prof. Marko Gerbec
  2. Asst. Prof. Evgeny Goreschnik
  3. Dr. Adolf Jesih
  4. Asst. Prof. Robert Kocjančič
  5. Dr. Zoran Mazej
  6. Prof. Maja Ponikvar-Svet
  7. Asst. Prof. Tomaž Skapin
  8. **Asst. Prof. Gašper Tavčar, Head**
  9. Dr. Melita Tramšek
- Postdoctoral associates**
10. Dr. Matic Lozinšek
- Postgraduates**
11. Blaž Alič, B. Sc.

12. David Levovnik, B. Sc.
  13. Dona Pavlovič, B. Sc.
  14. *Dr. Igor Shlyapnikov, left 30.03.16*
  15. Žiga Zupanek, B. Sc.
- Technical officers**
16. Peter Frkal, B. Sc.
  17. Tine Oblak, M. Sc.
  18. Tomaž Ogrin, M. Sc.
- Technical and administrative staff**
19. Pero Kolobaric
  20. Robert Moravec
  21. Mira Zupančič

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## SHORT ARTICLE

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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# DEPARTMENT OF PHYSICAL AND ORGANIC CHEMISTRY

# K-3

**The basic research of the department is focused on the experimental and theoretical study of various physico-chemical processes at surfaces and in atmospheric chemistry. The main attention in the field of organic chemistry is directed to green chemical approach to transformation of organic compounds.**

Experimental research in the field of electrochemistry is oriented to the protection of biomedical materials and modern types of corrosion protection for technological materials.

Our investigations were focused on the functional protection of biomedical materials, titanium-based and cobalt-chromium alloys, used for temporary bone and dental implants. The synthesis of fluoroapatite (FA) and fluorohydroxyapatite (FHA) was followed by *in situ* FTIR to determine the mechanism of sol formation. The initial triethyl phosphite precursor was hydrolyzed to phosphate after the addition of ammonium fluoride and calcium nitrate. Following the addition of calcium nitrate, the process proceeded at a higher temperature and a slightly alkaline pH to achieve the formation of the final sols. Depending on the amount of ammonium fluoride added, fluoroapatite or fluorohydroxyapatite sol gels resulted. Both types of coating were macroscopically dense and uniform, consisting of nano-sized particles. The microstructures of both FHA and FA coatings are the same as that for hexagonal calcium phosphate fluoride, as shown by X-ray diffraction. Both fluoroapatite and fluorohydroxyapatite coatings performed better than an uncoated CoCrMo substrate in Fusayama artificial saliva that simulates dental applications. The coatings exhibit the hydrophilic behaviour that is recommended for osteoblast differentiation in tissue engineering. The present work demonstrates the possibility of applying fluoroapatite and fluorohydroxyapatite coatings to a CoCrMo substrate, thus increasing the functional ability of the substrate for osseointegration.

Another paper is focused on the elaboration of ZrO<sub>2</sub> films on pure zirconium via anodizing in phosphoric acid with and without fluoride at constant potentials of 30 V and 60 V. The structure and composition of the films were investigated using scanning electron microscopy, Raman spectroscopy and X-ray photoelectron spectroscopy. The composition of the oxides formed at both potentials can be identified as monoclinic ZrO<sub>2</sub>. In addition to Zr and O, layers formed in phosphoric acid contain phosphorus originating from phosphoric acid. When the phosphoric acid solution contains NaF, fluorine is also incorporated in the oxide layer. Anodized samples exhibit smaller current densities during anodic polarization in artificial saliva compared to the as-received zirconium covered with *native* oxide. The surface treatment achieved by anodizing Zr at 60 V in the mixture of phosphoric acid and NaF seems to be the most promising from the point of view of corrosion behaviour. Further studies regarding the bioactivity of this alloy with the optimal surface treatment should be conducted.

Sol-gel TiO<sub>2</sub> and Ag-TiO<sub>2</sub> coatings were synthesized and deposited on a titanium substrate by spin-coating in order to increase the functionality of the surface for biomedical applications. Synthesis under acidic conditions using TiCl<sub>4</sub>, HCl and H<sub>2</sub>O<sub>2</sub> resulted in the formation of TiO<sub>2</sub> with predominantly rutile microstructure according to the X-ray diffraction data. Its morphology is homogeneous and dense. The addition of AgNO<sub>3</sub> to the synthesis route results in the formation of Ag-TiO<sub>2</sub>. Spherical particles are nano-sized and present throughout the coating surface. The silver particles shift the absorption of TiO<sub>2</sub> to the visible region, as shown by UV/Vis spectroscopy. This eliminates the need for the UV illumination of TiO<sub>2</sub> in order to activate its antibacterial ability.



Head:  
**Prof. Ingrid Milošev**

**Sol-gel routes were demonstrated as desirable routes for tailoring materials with functional properties suitable for biomedical materials: corrosion protection, osseointegration ability and antibacterial properties.**

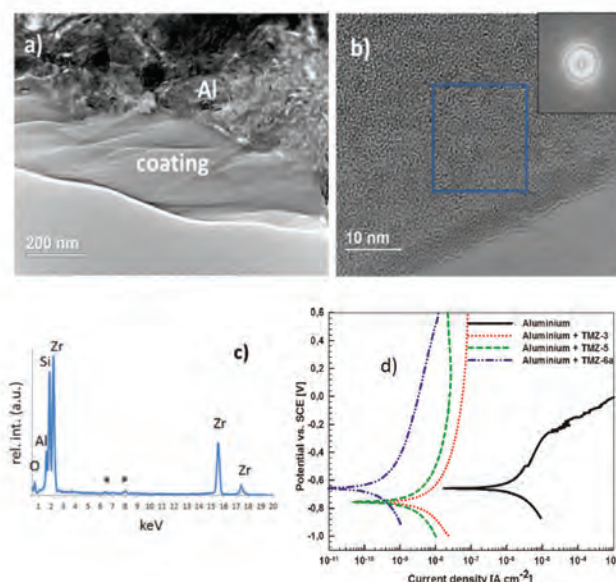


Figure 1: (a) Bright-field transmission electron micrograph (BF-TEM) of TMZ-6a\* hybrid amorphous sol-gel coating on aluminium, (b) high-resolution TEM micrograph of coating with the corresponding Fast Fourier Transform (FFT) the marked region, (c) TEM-EDXS (Energy-dispersive X-ray spectroscopy) pattern obtained from the coating, peaks denoted by \* are due to TEM holder, (d) potentiodynamic polarization curves measured in simulated aircraft conditions (Harrison's solution, 0.35% (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> + 0.05% NaCl) for uncoated aluminium and aluminium coated with TMZ-3, TMZ-5 and TMZ-6a coatings.  $dE/dt = 1$  mV/s.



Electrochemical polarization measurements of deposited coatings in simulated physiological solution confirm their protective properties, which are reflected in a larger polarization resistance and a smaller corrosion current density compared to uncoated titanium. The presence of Ag can be detected electrochemically by the peak at 0.11

**Cerium acetate salt is a suitable corrosion inhibitor for aluminium alloys, not only because its inhibitor efficiency, but also its ability to re-passivate and self-heal surface defects during immersion in chloride solution.**

V vs. Ag/AgCl electrode. This peak disappears after prolonged immersion (120 h), indicating the release of silver particles. The latter process does not affect the structural or protective properties of TiO<sub>2</sub> coatings, which retain a highly protective ability with resistance values in the MΩ cm<sup>2</sup> range, as confirmed by polarization and electrochemical impedance measurements. The antibacterial properties of deposited coatings were investigated in the presence of *Pseudomonas aeruginosa*, a biofilm forming bacteria. The

adhesion of bacteria is reduced on coated titanium in comparison to uncoated substrate. Although the difference was not statistically significant, the imaging of bacteria after exposure to coated surfaces clearly shows the destruction of the 'spherical' bacteria shape and leaching of the cell interior. Therefore, the coatings, especially those containing silver particles, express antibacterial ability that is mainly related to morphological changes and destruction of bacteria cells. The presence of silver in TiO<sub>2</sub> coatings prepared in this work is not cytotoxic to human osteoblastoma cells. The presented coatings offer the potential for use in biomedical applications.

In the area of technological materials we were concentrated primarily on alloys based on aluminium. Aluminium alloys are widely used in different industries and are one of most

important materials today, especially in transportation industry due to the need to reduce vehicle weight and, consequently, to reduce the fuel consumption. Traditional ways of corrosion protection of aluminium alloys, i.e., chromate coatings, are not applicable due to ecological restrictions. In the last decade numerous alternatives are being explored, among which the most important are sol-gel coatings, conversion coatings and inorganic and organic inhibitors. In our laboratory all alternatives are being investigated and even combined with each other, i.e., sol-gel and inhibitors, in order to achieve not only a barrier type of protection but active protection, aiming to self-heal the corrosion damage at the surface. We were particularly successful in the development of hybrid sol-gel coatings comprising tetraethyl orthosilicate (TEOS), 3-(trimethoxysilyl)propyl methacrylate (MAPTMS) and zirconium(IV) propoxide (ZTP). The contents of ZTP and methacrylic acid (MAA) have an important influence on the ageing process, which was studied using dynamic light scattering. Sols with smaller amounts of MAA and ZTP stabilized more slowly, which was more suitable for subsequent deposition. Coatings are amorphous, as shown by transmission electron microscopy. Thus, the synthesis leads to the incorporation of zirconium into an inorganic-organic silicon oxide matrix and not to the formation of ZrO<sub>2</sub> nanoparticles. The hydrophobic character of the coating increases with increasing molar content of ZTP and MAA. Two-component sol-gel

synthesis thus enables a relatively simple procedure for the production of hybrid coatings with properties that can be tailored depending on the composition of the sol and conditions of ageing and curing. The obtained properties, amorphous structure, homogeneity and low wettability are the basis for their use in corrosion protection, which was tested under simulating aircraft conditions.

Another alternative to chromate coatings are rare-earth salts (cerium and lanthanum) used either as corrosion inhibitors added to solution or as conversion coatings. When added as inhibitors, the inhibitory actions on Al,

AA2024-T3 and AA7075-T6 of various cerium salts, Ce(III) chloride, Ce(III) nitrate, Ce(III) acetate and Ce(IV) sulphate, in 0.1 M NaCl were compared. Although in all cases protection is achieved by the deposition of cerium hydroxide on cathodic sites, the course of inhibition is dependent on the type of anion and on the substrate, i.e., the composition of intermetallic particles in the alloy. The inhibitory action of all cerium(III) salts was the greatest on AA7075-T6, followed by Al, and the smallest on AA2024-T3. The reason for this is interpreted in terms of the different compositions of

intermetallic particles in the particular alloy and of the dependence of corrosion protection on the type of anion and pH. The addition of the same concentration of different cerium(III) salts leads to different pHs, consequently affecting the stability, not only of the intermetallic particles, but also of the surrounding aluminium oxide matrix. Ce(III) acetate was the most effective inhibitor for all three materials studied, followed by Ce(III) nitrate and chlo-

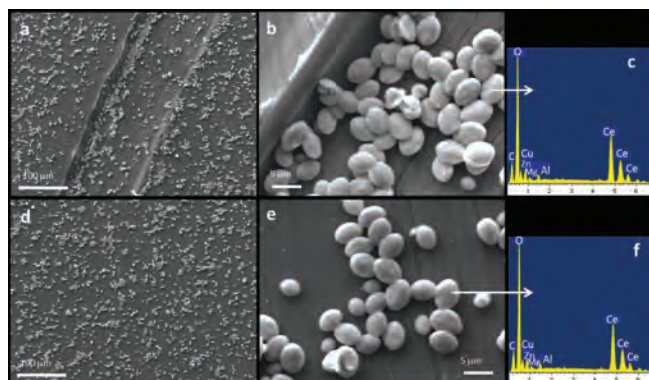


Figure 2: Scanning electron microscopy/energy-dispersive X-ray spectroscopy (SEM/EDS) analysis of the aluminium alloy 7075-T6 surface after 72 h scratch immersion test in 0.1-M NaCl containing 3 mM Ce(Ac)<sub>3</sub>. The samples were immersed for 24 h, scratched using a ceramic knife, and immersed for another 48 h. (a) SEM low secondary electron image at the scratch, (b) SEM compositional mode image and (c) EDS spectrum of the surface within the scratch showing deposits of cerium oxide, and (d) and (e) SEM low secondary electron image of the surface away from the scratch at (d) high and (e) low magnification showing deposits of cerium oxide, as shown by (f) EDS spectrum.

**We demonstrated that the surprising counter-intuitive attractive lateral interactions between negatively charged O adatoms on Al surfaces are a consequence of an electrostatic stabilization that stems from an interplay between ionic interactions and geometric effects.**

ride. This is reflected, not only in the increase in polarization resistance and decrease in corrosion current density, but also in the increase in resistance to pit nucleation. Long-term immersion testing confirmed the good corrosion-inhibition properties. Even after 2 months corrosion products were not formed, in contrast to uninhibited samples in which corrosion products were observed after 3 h. Cerium acetate is thus established as the best corrosion inhibitor for AA7075-T6 in a chloride medium, not only because of its good inhibition effectiveness but also because of its low price and lack of toxicity. Moreover, it enables the re-passivation of the surface defects, which was not observed in the case of cerium chloride.

In 2016 we started to work on the project COR\_ID within M-ERA.NET (European Research Area, an EU funded network). The main aim of the project “Design of corrosion resistant coatings targeted for versatile applications” (acronym COR\_ID) is to design and engineer new coatings for aluminium alloys with targeted properties of increased corrosion resistance, specific hydrophobic properties, prolonged service life-time and reduced ecological impact. Industry-driven needs will be solved using an integrated computational materials engineering (ICME) approach and produce economic material benefiting with increased market competitiveness. The project consortium, coordinated by Prof. Ingrid Milošev, comprises researchers from Slovenia, France and Hungary: Department of Physical and Organic Chemistry of the Jožef Stefan Institute, Talum d.d. Kidričevo (partner mag. Dejan Lorber), Chimie ParisTech (CNRS) from Paris (partner Prof. Philippe Marcus) and Eötvös Loránd University from Budapest (partner Prof. József Rábai). The project consortium links scientists from three partner countries and one technological company (Talum Kidričevo d.d.) aiming to stimulate advances in basic and applied research and technology transfer.

For the past several 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 reduced and oxidized surfaces of copper and to a smaller extent with reduced surfaces of iron. Our principal aim is to better understand how organic corrosion inhibitors act against corrosion at the molecular level and to discern the fundamental principles that govern their corrosion-inhibition characteristics. Recently, we also started to model the oxidation of aluminium surfaces. The oxidation of a metal generally begins with the dissociation of a molecular oxidizing agent. For oxidizing agents, such as  $O_2$ , this initially results in chemisorbed oxygen adatoms. It is known that during the adsorption of electronegative atoms on a more electropositive metal surface, charge transfer occurs and adatoms become negatively charged, typically resulting in repulsive lateral interactions. However, in the case of O on Al surfaces the opposite occurs and the lateral interactions between adatoms are attractive. Although this O/Al anomaly has been noticed, no sound explanation as to why this occurs has been given in the literature. We demonstrated that the surprising counter-intuitive attractive lateral interactions between negatively charged oxygen adatoms on Al surfaces are a consequence of an electrostatic stabilization that stems from an interplay between ionic interactions and geometric effects. Namely, for the high-coverage ( $1 \times 1$ ) overlayer the positive charge of surface Al ions is considerably larger compared to lower coverage situations, which strengthens the O–Al bonds. However, to take advantage of this effect, the adatoms have to be located close enough to the surface, i.e., there exists a critical adatom height above the surface, below which the lateral interactions are attractive and above which they are repulsive (see Figure 3). There is nothing specific to O and Al in this explanation and our calculations suggest that the model should be generally applicable, provided that (i) the adsorption bonding is sufficiently ionic and (ii) adatoms are sufficiently small to come close enough to the metal surface.

In the field of atmospheric chemistry the effect of water molecules on the direct hydrogen abstraction from HOSO by  $NO_2$  were investigated. The potential energy surface for naked reaction and for one or two water molecules catalysed reactions are qualitatively identical but shifted to more

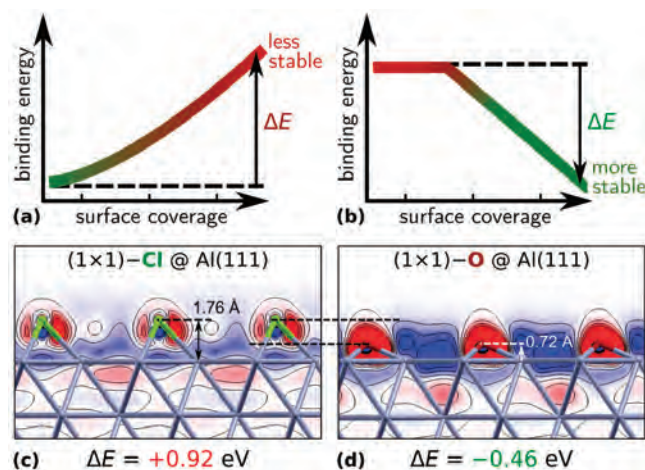


Figure 3: (a) Typical dependence of adatom binding energy on the surface coverage, i.e., the adatom–surface binding becomes less stable as the coverage increases due to repulsive lateral interactions between the adatoms; such a dependence is exhibited by Cl on Al(111). In contrast, for O adatoms on Al surfaces the opposite occurs and the lateral interactions between adatoms are attractive; the corresponding anomalous dependence of binding energy on the coverage is shown in (b). (Bottom) Charge density difference for Cl (left, c) and O (right, d) adatoms on Al(111) at high coverage. The blue colour represents the electron deficit regions, while the electron excess regions are coloured in red.

**The direct hydrogen abstraction from the HOSO radical by  $NO_2$  becomes barrier-less already in the presence of a single water molecule. The process is spontaneous and very feasible under tropospheric conditions, as well as at the combustion temperatures.**

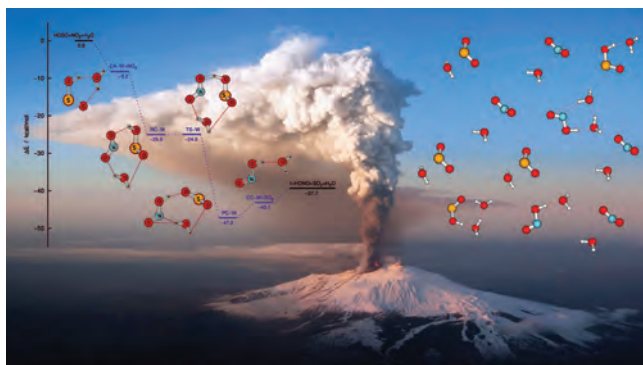


Figure 4: Water-mediated transformation of HOSO radical to HONO radical.

negative energies. The results demonstrate that the barrier for the direct hydrogen abstraction is low and the barrier for the one water-catalysed reaction decreases practically to zero. The second water molecules have no further effect either on the barrier height nor on the mechanism, thus, already in the presence of a single water molecule the hydrogen abstraction process becomes barrier-less. The process is spontaneous and very feasible under atmospheric conditions as well as at the combustion temperatures.

**Seven new masked analogues of phosphopantothenate, suitable for an evaluation of their potential ability to restore intracellular coenzyme A (CoA) levels, were successfully synthesized in good-to-moderate yields.**

Subsequent studies on the thermodynamic parameters for the deactivation of HOSO radical and its complexes with water and formic acid molecules in the reactions with the hydrogen atoms and the hydroxy radicals have shown that the complex transformations into the final products are less exothermic compared to the deactivation of the free radical. On the other hand, the Gibbs free energy changes remain almost the same due to the increased entropy contributions.

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

The new method for direct preparation of vicinal halohydrines or vicinal halo methoxy alkanes from tertiary phenyl substituted alcohols bearing at least one vicinal proton using N-halosuccinimides in aqueous or methanolic reaction media was developed.

We have continued the development of the new method of cross-coupling reaction between benzyl alcohols and phenyl-substituted alkenes catalysed by molecular iodine under solvent-free reaction conditions. The scope of the transformation resulting in the formation of 1-phenyl-2-benzylalkenes was comprehensively tested on a variety of benzyl alcohols and few examples of convenient alkenes.

Two new methods for the aerobic oxidation of alcohols have been discovered, tested and evaluated using fluoro alcohols as template catalysts.

Primary benzyl alcohols we selectively and efficiently transformed to aldehydes using the new reaction system oxygen/(cat.)HNO<sub>3</sub>/1,1,1,3,3,3-hexafluoropropan-2-ol (HFIP, solvent and template catalyst). Oxygen has the role of the terminal oxidant, HNO<sub>3</sub> is the oxidant and the source of nitrogen oxides, while the activation of the system was obtained by HFIP, which acts as a template catalyst and the reaction media. Its activation is high enough that no additional co-catalysis using metal ions or TEMPO derivatives was necessary. Secondary alcohols were selectively oxidised into ketones with no reaction on the primary alcohol group. Reactions were performed at room temperature with excellent yields. The oxidation of alcohols was catalysed by inexpensive and easily available FeCl<sub>3</sub> and HNO<sub>3</sub>. As the terminal oxidant O<sub>2</sub> was used. 1,1,1,3,3,3-hexafluoropropan-2-ol (HFIP) has a dual role as it works as a solvent as well as a template catalyst. HFIP can be easily recovered under reduced pressure. An explanation of the mechanism is proposed (Figure 5).

In the framework of 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 concluded and published the results of the development of new reagents for a phosphorylation of alcohols and one of them was successfully used on derivatives of pantothenic acid, which carry a

potential function as prodrugs of phosphates. We were developing new products used in non-human cosmetics for the company ECOT. In the Jožef Stefan International Postgraduate School we are performing two organic green-chemistry courses and at the Faculty for Chemistry and Chemical Technology at the University of Maribor a few undergraduate courses of organic chemistry

**Some outstanding publications in the past year**

1. P. Rodič, A. Mertelj, M. Borovšak, A. Benčan, D. Mihailović, B. Malič, I. Milošev, Composition, structure and morphology of hybrid acrylate-based sol-gel coatings containing Si and Zr composed for protective applications, *Surf. Coat. Technol.*, 286 (2016) 388-396
2. D. Covaciu Romonti, J. Iskra, M. Bele, I. Demetrescu, I. Milošev, Elaboration and characterization of fluoro-hydroxyapatite and fluoroapatite sol-gel coatings on CoCrMo alloy, *J. Alloys Compds*, 665 (2016) 355-364
3. M. Poberžnik, A. Kokalj, Origin of surprising attractive interactions between electronegative oxygen atoms on aluminium surfaces, *J. Phys. Chem. C*, 120 (2016), 25915-25922

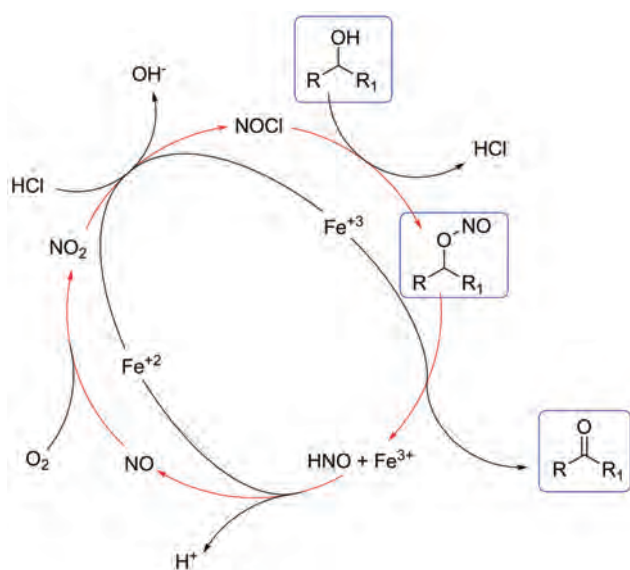


Figure 5: The proposed reaction pathway of the aerobic oxidation of secondary alcohols using the reaction system oxygen/(cat.)FeCl<sub>3</sub>/(cat.)HNO<sub>3</sub>/hexafluoro isopropanol.

- S. Tušar, A. Lesar, Hydrogen bonding in the hydroxysulfinyl radical-formic acid-water system: a theoretical study, *J. Comput. Chem.*, 37 (2016), 1611-1625
- J. Pahor, S. Stavber, A. Čusak, G. Kosec, H. Petković, A. Podgoršek, Toward the efficient synthesis of new phosphopantothenate derivatives by using chlorophosphate reagents, *Synthesis*, 48 (2016), 3763-7881

### Awards and appointments

- Ingrid Milošev: Pregl Award for Exceptional Achievements in the field of chemistry and related disciplines
- Klara Čebular: IUPAC Poster Prize, on 6<sup>th</sup> International IUPAC Conference on Green Chemistry, Venice, Italy, September 2016

### Organization of conferences, congresses and meetings

- EUSpec COST Action MP1306, EWinS 2016: EUSpec Winter School on Core Level Spectroscopies, Ajdovščina, Slovenia, 1.2.-11.2.2016
- 4<sup>th</sup> CARISMA Meeting, CMST COST Action CM1205, Ljubljana, Slovenia, 21.3.-23.3.2016
- Kick-off Meeting, M-ERA.NET Project »COR\_ID«, Ljubljana, Slovenia, 11.4-12.4.2016
- Kick-off Meeting, M-ERA.NET Project »COIN DESC«, Ljubljana, Slovenia, 27.10.-28.10.2016

### Patent granted

- Rok Zupet, Jernej Iskra, Miloš Ružič, Anica Pečavar, Ivanka Kolenc, Jože Pucelj, Igor Plaper, A process for a preparation of marbofloxacin and intermediate thereof, EP2501680 (B1), European Patent Office, 10. 02. 2016

## INTERNATIONAL PROJECTS

- CARISMA; Catalytic Routines for Small Molecule Activation; CMST COST Action CM1205  
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
- Exploring Antimalarial Peroxides from Bench-side to Bed-side: Synthesis, Chemistry, Antimalarial Assessment and SAR studies of Novel functionalized 1, 2, 4-Trioxanes and 1, 2, 4, 5-Tetraoxanes against Multi-drug Resistant Malaria  
Prof. Jernej Iskra  
Slovenian Research Agency
- CECICORR - Computational Modeling and Experimental Characterization of Interfaces relevant for CORrosion: Passive Films and Corrosion Inhibitors  
Asst. Prof. Anton Kokalj  
Slovenian Research Agency
- Corrosion Protection of Technologically Important Materials using Environmentally-friendly Coatings  
Prof. Ingrid Milošev  
Slovenian Research Agency
- Study of the Synthesis of Bioactive Furans and their Inhibitory Role in Antimicrobial Hybrid Coatings  
Prof. Jernej Iskra  
Slovenian Research Agency

## RESEARCH PROGRAMS

- Chemistry for sustainable development  
Prof. Stojan Stavber
- Advanced materials for low-carbon and sustainable society  
Prof. Ingrid Milošev

## R & D GRANTS AND CONTRACTS

- 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  
Prof. Jernej Iskra
- New technology for design of novel polyketide drug-leads with chemically amenable moieties  
Prof. Stojan Stavber
- COR\_ID: Design of corrosion resistant coatings targeted for versatile applications  
Prof. Ingrid Milošev
- Small Services  
Prof. Ingrid Milošev

## VISITORS FROM ABROAD

- Prof. dr. Lorenzo Fedrizzi, University of Udine, Italy, 18.5.-18.5.2016
- Gregor Ekart, B.Sc. student. Imperial College London, England, 4.7.-8.9.2016
- Dominique Costa, Chemie Paris Tech, Ecole Nationale Supérieure de Chimie de Paris, Paris, France, 19.12.-23.12.2016
- Dr. Bojan Božič, University of Belgrade, Faculty of Technology and Metallurgy, Serbia, 1.10.-31.12.2016

## STAFF

### Researchers

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

### Postdoctoral associates

- Dr. Tina Bakarič
- Dr. Peter Rodič

### Postgraduates

- Dunja Gustinčič, B. Sc.
- Dr. Jerca Pahor, left 01.08.16

- Matic Poberžnik, B. Sc.
- Griša Grigorij Prinčič, B. Sc.
- Dr. Katarina Starkl Renar, left 01.06.16
- Gavrilko Sekularac, B. Sc.
- Urša Tiringner, B. Sc.
- Dr. Simona Tušar, left 01.06.16
- Barbara Volarič, B. Sc.

### Technical officers

- Barbara Kapun, B. Sc.

Note:

\* part-time JSI member

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# ELECTRONIC CERAMICS DEPARTMENT

K-5

***The Electronic Ceramics Department is active in the research of the synthesis, properties and applications of materials for electronics and energetics, mainly complex multifunctional materials and structures that can perform multiple functions (multifunctional materials). The materials of interest include ceramic piezoelectrics, ferroelectrics, relaxors, multiferroics and conductive oxides. The emphasis is on the creation of the properties by the synthesis and structure on the nano-, micro- and macro-levels. The group also works on the principles of the 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. In collaboration with the National Institute of Chemistry, University of Ljubljana, University of Nova Gorica, Montanuniversität Leoben, Austria, and the University of Milan, Italy, we explained the mechanism of grain-growth inhibition in perovskite ceramics due to the addition of an aliovalent dopant for the case of strontium-doped ceramic  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$  (KNN). The investigations of highly doped samples suggested that the system tends to segregate the A-site vacancies, which occur as a result of doping, in a secondary phase. Together with increasing lattice disorder and microstrain, these effects are correlated with the increasing number of low-angle grain boundaries, which finally limit the grain growth and consequently result in a significant grain-size decrease. Furthermore, the effect of the Sr dopant on the solid-state synthesis of KNN was studied by thermal analysis and in-situ high-temperature X-ray diffraction. Strontium doping had an insignificant influence on the course of the solid-state synthesis. On the other hand, the particle size distribution of the  $\text{Nb}_2\text{O}_5$  reagent proved to be a crucial factor influencing the temperature interval of the KNN solid-state synthesis.

Within the activities on **lead-based piezoelectric ceramics**, we studied the ferroelectric domain structure of the  $\text{Pb}(\text{Sc}_{0.5}\text{Nb}_{0.5})\text{O}_3$  ceramics, prepared by mechanochemical activation of powder, by piezoresponse force microscopy. Micrometre-sized domains with different morphologies exist in the material at room temperature. Slightly below the ferroelectric-relaxor phase transition, i.e., at 90 °C, the fraction of micrometre-sized domains is reduced, while the nanometre-sized domains prevail in accordance with the ferroelectric-relaxor crossover at ~98°C.

The tilting of oxygen octahedra in perovskites has been proposed to profoundly affect the macroscopic domain switching behaviour in undoped, rhombohedral  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  (PZT) ceramics, resulting in pinched ferroelectric hysteresis loops. A similar effect, however, is expected because of the presence of defect complexes involving oxygen vacancies. We revisited the early studies on rhombohedral PZT ceramics revealing that the observed pinched loops are likely associated with the presence of defect complexes and not octahedral tilts, as previously suggested.

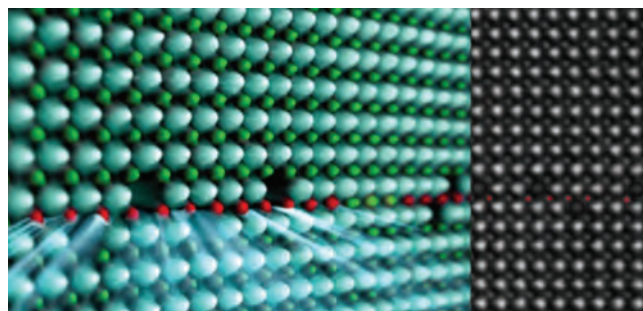
Within the 7 FP EU CERAMPOL project and in collaboration with our research partner HIPOT-RR, we fabricated an innovative **vibrating system for wastewater purification**. The system is based on a porous ceramic membrane that vibrates under the influence of an electrically-driven PZT piezoelectric integrated into the membrane. We optimised the system's operation conditions using finite-element modelling and measurements of the displacement amplitudes of the system in a wide frequency range. We demonstrated with tests under real operating conditions that the novel vibrational system can be effectively used for water purification. With the project partner LEITAT, Spain, we submitted a PCT patent application.

Within the activities on **multiferroic ceramic  $\text{BiFeO}_3$** , in cooperation with colleagues from the Department of Advanced Materials, Department of Inorganic Chemistry and Technology, National Institute of Chemistry, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland and the University of Shizuoka, Japan, we studied the mechanism of domain con-



Head:  
**Prof. Barbara Malič**

**Researchers from the “Jožef Stefan” Institute and National Institute of Chemistry, in collaboration with colleagues from Switzerland and Japan, were the first to identify the accumulation of charged defects at domain walls in ferroelectric  $\text{BiFeO}_3$ . This finding explains the conduction at the domain walls in  $\text{BiFeO}_3$  and thus represents the missing piece for explaining the intriguing electrical properties of domain walls in ferroelectrics. The study was published in Nature Materials, currently one of the highest-impact scientific journals.**



*Figure 1: Artistic presentation of accumulated defects at a domain wall in  $\text{BiFeO}_3$  (painter Mito Gegič) and image of bismuth (larger) and iron (smaller) atomic columns taken with a scanning transmission electron microscope.*



ductivity in ferroelectric BiFeO<sub>3</sub>. We were the first to identify the accumulation of charged defects at domain walls in ferroelectric BiFeO<sub>3</sub>. This finding explains the p-type hopping conduction at the domain walls in BiFeO<sub>3</sub>. The study was published in Nature Materials with a 2015 impact factor of 38.89, which currently makes it one of the highest-impact scientific journals. (Figure 1)

BiFeO<sub>3</sub>-based ferroelectric solid solutions suffer from a high electrical conductivity, which represents one of the major obstacles for the use of these materials in high-temperature piezoelectric applications. We investigated this problem in BiFeO<sub>3</sub>-SrTiO<sub>3</sub> ceramics and thus developed ways for controlling the electrical conductivity by annealing ceramics in different atmospheres. An alternative approach using manganese as a dopant has not only eliminated the original high conductivity but also stabilized the decreased conductivity against subsequent annealing in air and by the application of elevated electric fields.

The electrocaloric (EC) effect is defined as the adiabatic and reversible temperature change that occurs in a polar material upon the application of an external electric field. In collaboration with the Condensed Matter Physics Department and Laboratory for Refrigeration and District Energy, Faculty of Mechanical Engineering, University of Ljubljana, we analysed the energy efficiency of an EC cooling system in view of the polarization–electric field (*P* – *E*) hysteresis losses of the EC materials, and recovery of the electric energy needed to induce the EC effect. We showed that the energy efficiency of the materials with large hysteresis losses, i.e., 100(1-x)Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>–100xPbTiO<sub>3</sub> (PMN-100xPT) compositions close to the morphotropic phase boundary, i.e., PMN-35PT, is significantly reduced as compared to the PMN-rich relaxor compositions. Therefore, we proposed that the EC materials with low *P* – *E* hysteresis losses, such as PMN-100xPT with x≤0.1, and a high degree of the electric-energy recovery should be implemented in an EC cooling system in order to achieve a high energy efficiency.

Electric-field amplitudes needed to reach EC temperature changes ( $\Delta T$ ), suitable for applications in cooling technology, that is at least 2K, are close to the dielectric breakdown strength of respective bulk ceramic materials, typically about 100 kV/cm. In order to reduce the applied voltage for a given EC  $\Delta T$ , we prepared **multilayer cooling elements** of relaxor ferroelectric 0.9Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>–0.1PbTiO<sub>3</sub> (PMN-10PT) with internal platinum electrodes by tape-casting and lamination in collaboration with the company KEKO-Equipment, Žužemberk. The thickness of the individual layers was about 60  $\mu$ m. The EC temperature changes of multilayer elements were measured between 55 and 105 °C at electric field amplitudes of up to 100 kV/cm in a high-resolution calorimeter. The highest EC  $\Delta T$  was 2.26 K at 100 kV/cm at 105 °C. The obtained result is in good agreement with

the values obtained in the bulk ceramic of the same composition with typical thicknesses exceeding 100  $\mu$ m, but it was obtained at a much lower applied voltage, thus presenting another step towards the application of EC ceramic materials in solid-state cooling.

Using the finite-element method we modelled the behaviour of an EC solid-state cooler for its possible use in microelectronics. The essential parts of the cooler are multifunctional **cantilevers** fabricated from PMN-10T, which exhibit simultaneous bending and change of temperature upon the application of an electric field. The results of the modelling confirmed that by introducing thermal contacts between the cantilevers a temperature gradient is formed across the structure, resulting in a promising cooling capacity.

Furthermore, we prepared a **multicaloric ceramic material** 0.8Pb(Fe<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub>–0.2Pb(Mg<sub>1/2</sub>W<sub>1/2</sub>)O<sub>3</sub> that shows both an electrocaloric and a magnetocaloric temperature change. The work is the first experimental confirmation of the electrocaloric and magnetocaloric coexistence in relaxor-ferroelectric and opens up new possibilities in the field of caloric cooling (Figure 2)

In the frame of the M-ERA.NET PiezoMEMS project we continued the research of ferroelectric thin films based on lead-free perovskites for piezoelectric energy-harvesting applications together with partners from Poland and Romania. The influence of donor doping on microstructure, ferro- and piezoelectric properties of K<sub>0.5</sub>Na<sub>0.5</sub>NbO<sub>3</sub> films was studied.

In collaboration with LETI, Grenoble, France, Faculty of Physics, Vilnius University, Lithuania, School of Electronic and Information Engineering, Xi'an Jiaotong University, China, and the Condensed Matter Physics Department, JSI, we investigated the dielectric properties of Ba<sub>0.5</sub>Sr<sub>0.5</sub>TiO<sub>3</sub> (BST) thin films on alumina substrates with film thicknesses between 90 nm to 600 nm

**Researchers from the “Jožef Stefan” Institute, in collaboration with colleagues from Poland and South Korea, prepared a multicaloric 0.8Pb(Fe<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub>–0.2Pb(Mg<sub>1/2</sub>W<sub>1/2</sub>) material. The work is the first experimental confirmation of the electrocaloric and magnetocaloric coexistence in relaxor-ferroelectric and opens up new possibilities in the field of caloric cooling. The article was published in the journal Scientific Reports.**

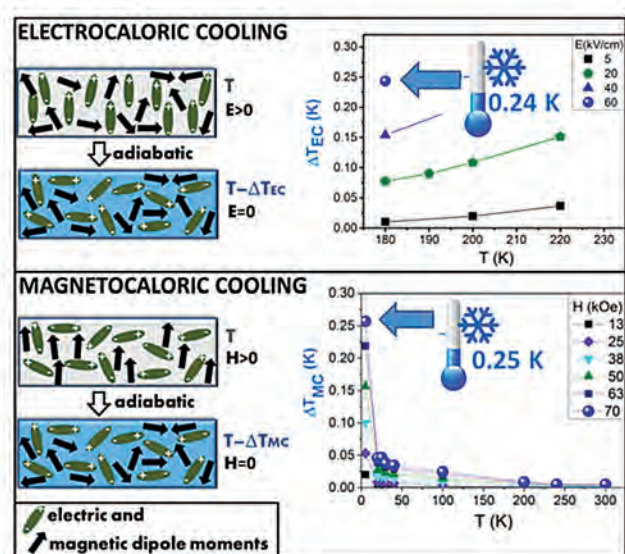


Figure 2: Multicaloric properties of 0.8Pb(Fe<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub>–0.2Pb(Mg<sub>1/2</sub>W<sub>1/2</sub>) material.

and predominantly columnar microstructures. The dielectric permittivity measured at room temperature exhibited a non-monotonous thickness dependence that was connected to the residual biaxial stress, developed in the BST films due to the thermal expansion mismatch between the film and the substrate. The dielectric permittivity of 170-nm-thick films with 75-nm-sized grains was 1180 measured at 5 kHz, which is one of the highest reported values for BST films with similar microstructures.

By understanding the influence of different thermal expansion coefficients of the thick film and the substrate and by controlling the chemical interactions between them, we successfully prepared by screen printing a few-10- $\mu\text{m}$ -thick films of bismuth ferrite ( $\text{BiFeO}_3$ ) with appropriate phase composition and microstructure. Bismuth ferrite is difficult to pole because it requires the use of high external electric field. We suggested an alternative way of poling by sintering the  $\text{BiFeO}_3$  films at a temperature above the ferroelectric-paraelectric phase transition. The presence of a compressive strain gradient across the film thickness cooled from above the ferroelectric-paraelectric phase transition was experimentally confirmed and was suggested to be responsible for the self-poling effect. These self-poled films exhibited a microstructure with randomly oriented columnar grains. (Figure 3)

We investigated the preparation of environmentally friendly thick-film piezoelectrics based on  $\text{K}_{0.5}\text{Na}_{0.5}\text{NbO}_3$  on metallic substrates by the electrophoretic deposition method.

We prepared  $\text{Pb}(\text{Zr,Ti})\text{O}_3$ -based thick-film structures by inkjet printing. We dispersed the ceramic powder in water and afterwards adjusted the viscosity and surface tension of the ink to be suitable for printing. We prepared arrays of linear structures with a line width of  $\sim 80\ \mu\text{m}$  and a micrometre-sized distance between the lines. After sintering at  $850\ ^\circ\text{C}$  the  $20\text{-}\mu\text{m}$ -thick structures exhibited a dielectric permittivity of 1100 and dielectric losses of 0.057, which are comparable to the properties of thick films prepared using screen-printing technology.

We inkjet printed high-K dielectric tantalum-aluminium-silicon-oxide nanostructures on indium-tin-oxide-coated glass as components for transparent electronics. The ink formulations with 2-methoxyethanol as the main solvent and highly viscous glycerol and/or 1,3-propanediol co-solvents exhibited the optimal values of the viscosity and surface tension for piezoelectric inkjet printing. By a suitable combination of all solvents in the ink the coffee-stain effect of the printed nanostructures could be avoided. We printed about 40-nm-thick, flat and uniform transparent capacitors with a good dielectric permittivity of  $\sim 15$ ,  $\tan(\delta) \sim 0.034$  at 100 kHz and a low leakage current density of  $2.4 \times 10^{-7}\ \text{A cm}^{-2}$  at  $200\ \text{kV cm}^{-1}$ . The study was performed in collaboration with the Condensed Matter Physics Department and the Department of Thin Films and Surfaces. (Figure 4)

In the framework of p-type semiconductors, the mechanism of formation of nanocrystalline  $\text{Co}_3\text{O}_4$  powder by cobalt nitrate-glycine solution combustion synthesis was studied. By controlling the reaction conditions and by using the sub-stoichiometric amount of glycine we prepared phase-pure  $\text{Co}_3\text{O}_4$ . The prepared powder contained soft cauliflower-shaped agglomerates with a high specific surface area ( $64.4\ \text{m}^2/\text{g}$ ). In collaboration with researchers from Eberhard Karls University of Tübingen, Germany, thick-film sensors were produced from the respective powder by drop-coating. The sensor annealed at  $600\ ^\circ\text{C}$  showed an excellent sensing performance for acetone detection at a low operating temperature of  $150\ ^\circ\text{C}$  in a humid environment. Such a sensor would be suitable for the detection of diabetes in exhaled air. (Figure 5)

We continued investigations of LTCC (Low Temperature Co-fired Ceramics) and thick-film materials and processes, used for fabrication of three-dimensional structures for different micro-electro-mechanical systems (MEMS) and chemical microsystems. The traditional co-operation with our research partners HIPOT-RR and Centre of Excellence NAMASTE



Figure 3: Distribution of the crystallographic orientations in columnar grains in thick  $\text{BiFeO}_3$  film with pronounced domain structure.

**Danijela Kuščer Hrovatin and Janez Holc, together with colleagues from ETI Elektroelement, Izlake, received a Silver recognition for the invention "Non-porous C410 cordierite materials for electrotechnics" by the Regional Chamber of Commerce Zasavje in June 2016.**

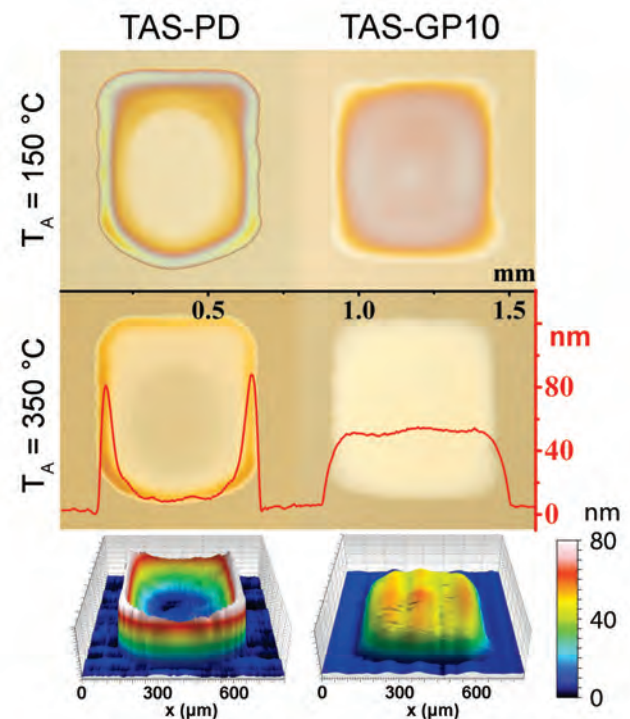


Figure 4: Optical images of the dried ( $150\ ^\circ\text{C}$ ) and heated ( $350\ ^\circ\text{C}$ ) inkjet-printed tantalum-aluminium-silicon oxide (TAS) based thin-film capacitors and the corresponding profilometry micrographs. By optimizing the TAS-ink formulation from 1,3-propanediol (PD)-based to a mixture of PD and glycerol (GP10) nano-structures with a uniform thickness of about 40 nm could be patterned.

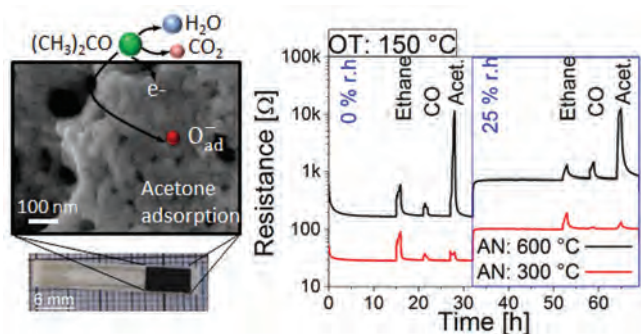


Figure 5: Image of a sensor surface of the active  $\text{Co}_3\text{O}_4$  layer taken with a scanning electron microscope with the schematic representation of acetone adsorption (left). DC resistance of sensors annealed at 300 and 600 °C, during exposure to ethanol (Ethane), carbon monoxide (CO) and acetone (acetyl) at an operating temperature of 150 °C in dry and humid environments (right). Cooperation with Eberhard Karls University, Tübingen.

continued resulting in several test structures and demonstration products. Examples include microfluidic components for electrochemical sensors and ceramic packaging for piezoelectric elements in the frame of INTcerSEN and PiezoMEMS projects, respectively, both from the M-ERA.NET programme, and pressure sensors designed as demonstration products from LTCC tapes developed by the company KEKO equipment.

In collaboration with the company ETI Elektroelement d.d., Izlake, we studied the manufacturing of the non-porous cordierite ceramic, which is used in products exposed to high-temperature differences in short periods of time. The material is suitable for automatic, large-scale production.

### Some outstanding publications in the past year

1. Rojac, Tadej, Benčan, Andreja, Dražič, Goran, Sakamoto, Naonori, Uršič, Hana, Jančar, Boštjan, Tavčar, Gašper, Makarovič, Maja, Walker, Julian, Malič, Barbara, Damjanovič, Dragan. Domain-wall conduction in ferroelectric  $\text{BiFeO}_3$  controlled by accumulation of charged defects. *Nature materials*, ISSN 1476-1122, [in press] 2016, 7 str., doi: 10.1038/nmat4799.
2. Khomyakova, Evgeniya, Šadl, Matej, Uršič, Hana, Daniels, John, Malič, Barbara, Benčan, Andreja, Damjanovič, Dragan, Rojac, Tadej. Self-poling of  $\text{BiFeO}_3$  thick films. *ACS applied materials & interfaces*, ISSN 1944-8244. [Print ed.], 2016, vol. 8, no. 30, str. 19626-19634, doi: 10.1021/acsami.6b05885.
3. Uršič, Hana, Bobnar, Vid, Malič, Barbara, Filipič, Cene, Vrabelj, Marko, Drnovšek, Silvo, Younghun, Jo., Wencka, Magdalena, Kutnjak, Zdravko. A multicaloric material as a link between electrocaloric and magnetocaloric refrigeration. *Scientific reports*, ISSN 2045-2322, 2016, vol. 6, str. 26629-1-26629-5, doi: 10.1038/srep26629.
4. Matavž, Aleksander, Frunza, Raluca-Camelia, Drnovšek, Aljaž, Bobnar, Vid, Malič, Barbara. Inkjet printing of uniform dielectric oxide structures from sol-gel inks by adjusting the solvent composition. *Journal of materials chemistry. C, Materials for optical and electronic devices*, ISSN 2050-7526. [Print ed.], 2016, vol. 4, no. 24, str. 5634-5641, doi: 10.1039/C6TC01090C.
5. Kuščer, Danjela, Bernardo, Mara, Santo-Zarnik, Marina, Malič, Barbara. Patterning of lead-zirconate-titanate thick-film structures by electrophoretic deposition from ethanol-based dispersions. *Journal of the European ceramic society*, ISSN 0955-2219. [Print ed.], 2016, vol. 36, no. 2, str. 291-297, doi: 10.1016/j.jeurceramsoc.2015.08.033.

### Awards and Appointments

1. Darko Belavič: Elected to the serving member of Electrotechnical Association Slovenia, MIDEM – Proposer: Society For Microelectronics, Electronic Components And Materials, Ljubljana, Slovenia May, 2016
2. Ines Bantan, Joži Prašnikar, Helena Razpotnik from ETI d.d., Danjela Kuščer, Janez Holc, from JSI, Electronic ceramics department K-5: Silver Award for innovation: “Neporozni kordieritni material C410 za elektrotehniko”, Gospodarska zbornica Slovenije, Zasavje, Slovenia, June 8, 2016
3. Lovro Fulanovič: SHAPING VI, Student poster award winner, Montpellier, France, July 20, 2016
4. Andraž Bradeško: Best poster award, Institute of Electrical and Electronics Engineers (IEEE), ISAF/ECAPD/PFM Conference 2016 – IEEE, Darmstadt, Germany, August, 21-25, 2016
5. Tomaž Kos, Tadej Rojac (co-mentor): Prešeren’s Award, Faculty of Electrical Engineering, Ljubljana, Slovenia, December 6, 2016

### Organization of Conferences, Congresses and Meetings

1. MIDEM 2016: 52<sup>nd</sup> International Conference on Microelectronics, Devices and Materials with the Workshop on Terahertz and Microwave Systems, Ankaran Slovenia, September 28-30, 2016
2. COST TO-BE Fall Meeting 2016, Ljubljana, Slovenia, September 28-30, 2016

## INTERNATIONAL PROJECTS

1. Feasibility Study and Fabrication of LTCC based PCB Multilayer  
Prof. Barbara Malič  
Ctr Carinthian Tech Research Ag
2. Fabrication of LTCC SAW Module Package and Plates  
Prof. Barbara Malič  
Ctr Carinthian Tech Research Ag
3. 7FP - CERAMPOL; Ceramic and Polymeric Membrane for Water Purification of Heavy Metal and Hazardous Organic Compound  
Asst. Prof. Danjela Kuščer Hrovatin  
European Commission
4. COST MP1308; Towards Oxide Based Electronics (TO-BE)  
Dr. Katarina Vojisavljević  
Cost Office
5. Functional Heterogeneity in Complex Oxides: Chemical Clustering, Atomic Displacements, and Polar Nanoregions  
Asst. Prof. Hana Uršič Nemevšek  
Slovenian Research Agency
6. Fabrication and Modelling of Integrated Piezoelectric Structures for High-frequency Ultrasound Applications  
Asst. Prof. Danjela Kuščer Hrovatin  
Slovenian Research Agency
7. Piezoelectric Films for Microelectromechanical Systems Based on Environment Friendly Perovskite Materials  
Prof. Barbara Malič  
Slovenian Research Agency

## RESEARCH PROGRAM

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

## R & D GRANTS AND CONTRACTS

1. Nanostructures for high-efficiency solar cells and photovoltaic  
Prof. Barbara Malič
2. New advanced electrocaloric materials for novel environmentally-friendly dielectric refrigeration technology  
Prof. Barbara Malič
3. Multifunctional materials for actuator and cooling devices  
Asst. Prof. Tadej Rojac
4. Photovoltaic cell and modul inhomogeneity analysis and performace monitoring in power plants through lifetime  
Prof. Barbara Malič
5. Tunable ferroelectric thin film capacitors for agile microwave antennas  
Prof. Barbara Malič
6. High-performance piezoelectric materials for sensors and actuators in high-temperature applications  
Asst. Prof. Tadej Rojac
7. Micro-electromechanical and electrocaloric layer elements  
Prof. Barbara Malič
8. Advanced electrocaloric energij conversion  
Prof. Barbara Malič
9. Integrated sensors with microfluidic features using LTCC technology  
Asst. Prof. Hana Uršič Nemevšek  
Piezoelectric MEMS for efficient energy harvesting  
Prof. Barbara Malič

## NEW CONTRACTS

1. Research of compatibility of LTCC materials and conductive pastes, with the emphasis on appropriate adhesion of the conductive material on LTCC and on simultaneous densification of both materials  
Prof. Barbara Malič  
Keko - Oprema d. o. o. Žužemberk

## VISITORS FROM ABROAD

1. Hugo Mercier, Université François-Rabelais de Tours, Tours, France, 1. Januar-8. October 2016
2. Mag. Stjepan Golubić, Visoka Tehnička Škola u Bjelovaru, Bjelovar, Croatia, 18. January 2016
3. Alen Britvić, Visoka Tehnička Škola u Bjelovaru, Bjelovar, Croatia, 18. January-18. April 2016
4. Dr. Carmen Galassi, Istituto di Scienza e Tecnologia dei Materiali Ceramici (ISTEC), Consiglio Nazionale delle Ricerche (CNR); Faenza, Italy, 16.-18. March 2016
5. Prof. Franck Levassort, Université François-Rabelais de Tours, Tours, France, 16.-18. March 2016
6. Alexandre-Benoît Bourgoin, Université de y of Limoges, Limoges, France, 2. April-31. July 2016
7. Dragana Vasiljević, Univerzitet ua v Novoem Sadu, Novi Sad, Serbia, 3.-23. April 2016
8. Jelena Vukmirović, Univerzitet ua v Novoem Sadu, Novi Sad, Serbia, 3.-23. April 2016
9. Prof. dr. Hisao Suzuki, Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan, 16.-18. April 2016
10. Prof. dr. Jacob L. Jones, North Carolina State University, Raleigh, US, 19.-22. June 2016
11. Dr. Vincenzo Buscaglia, Consiglio Nazionale delle Ricerche - IENI, Genova, Italy, 20.-22. June 2016
12. Prof. dr. Tomoya Ohno, Department of Materials Science, Kitami Institute of Technology; Kitami, Japan, 30. June-1. July 2016
13. Prof. Naonori Sakamoto, Research Institute of Electronics and Materials Science Course Department of Engineering, Graduate School of Integrated Science and Technology, Shizuoka University, Shizuoka, Japan, 30. June-8. July 2016
14. Mateusz Firynowicz, Politechnika Poznańska, Poznań, Poland, 4. July-10. October 2016
15. Anna Włodarkiewicz, Politechnika Poznańska, Poznań, Poland, 13. July-22. September 2016
16. Prof. Klaus Reichmann, Technische Universität Graz, Graz, Austria, 20. July 2016
17. Dong Hou, North Carolina State University, US, 29. August-3. September 2016
18. Reyhan Eşiyok, Yıldız Teknik Üniversitesi - Istanbul, Istanbul, Turkey, 1. September-26. November, 2016
19. Dr. Theodor Schneller, RWTH Aachen, Institut für Werkstoffe der Elektrotechnik II, RWTH Aachen, Aachen, Germany, 18.-20. September 2016
20. Mihael Štefić, Visoka Tehnička Škola u Bjelovaru, Bjelovar, Croatia, 26. September-23. December, 2016
21. Prof. Anatoliy Panich, Southern Federal University, Rostov-on-Don, Russia, 24. October 2016
22. Dr. Julian Walker, Pennsylvania State University, USA, 27.-28. October 2016
23. Agnieszka Monika Paszkowska, Uniwersytet Marii Curie-Skłodowskiej, Lublin, Poland, 24. October-31. December 2016
24. Karolina Szymanek, Uniwersytet Marii Curie-Skłodowskiej, Lublin, Poland, 24. October-31. December 2016
25. Dr. Denis Alikin, Ferroelectric Laboratory, Institute of Natural Sciences, Ural Federal University, Russia, 5.-18. November 2016
26. Assoc. Prof. Sverre Magnus Selbach, Norges teknisk-naturvitenskapelige universitet, Trondheim, Norway, 23.-25. November 2016
27. Krunoslav Kušec, Visoka Tehnička Škola u Bjelovaru, Bjelovar, Croatia, 19.-31. December 2016

## STAFF

### Researchers

1. Asst. Prof. Andreja Benčan Golob
2. Asst. Prof. Goran Dražić\*
3. Asst. Prof. Danjela Kuščer Hrovatin
4. **Prof. Barbara Malič, Head**
5. Asst. Prof. Tadej Rojac
6. Asst. Prof. Hana Uršič Nemevšek
7. Dr. Katarina Vojisavljević

### Postdoctoral associates

8. Dr. Mirela Dragomir
9. Dr. Kostja Makarovič\*
10. Dr. Mojca Otoničar
11. Dr. Tanja Pečnik
12. Dr. Marko Vrabelj

### Postgraduates

13. Andraž Bradeško, B. Sc.

14. Lovro Fulanović, B. Sc.

15. *Dr. Jitka Hreščak, 01.10.16, transferred to Department CEMM*

16. Dr. Evgeniya Khomyakova

17. Uroš Prah, B. Sc.

### Technical officers

18. Darko Belavič, B. Sc.

19. Silvo Drnovšek, B. Sc.

20. Brigita Kmet, B. Sc.

21. Maja Makarovič, B. Sc.

### Technical and administrative staff

22. Tina Ručigaj Korošec, B. Sc.

23. Matejka Smit, B. Sc.

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

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# DEPARTMENT FOR NANOSTRUCTURED MATERIALS K-7

*One of our biggest advantages is our interdisciplinary team. The basic and applied research of the Department for Nanostructured Materials includes metals, intermetallic alloys, biomaterials, ceramic materials, and minerals. Our research encompasses conventional processing as well as the development of new technologies and methods for preparing new materials with advanced properties. It includes experimental and theoretical investigations of structures, analyses of chemical compositions at the atomic level, and measurements and calculations of physical properties, all of which help us to improve the properties of micro- and nanostructured materials.*

## Magnetic Materials.

The European project MAG-DRIVE, coordinated by one of the members of the department, was successfully concluded. The research in MAG-DRIVE was focused on developing novel microstructural-engineering strategies that dramatically improved the properties of magnets based on light rare-earth elements, especially the coercivity, which enables them to be used for electric vehicle (EV) applications above 100°C. These magnets were also designed-to-recycle, with an emphasis on reducing conventional rare-earth magnets' need for easily oxidizing grain boundaries.

The European project REProMag entered its second year. The goal is to develop and validate an innovative resource-efficient manufacturing route for **rare-earth magnets** that allows for the economic and efficient production of net-shape magnetic parts with complex structures and geometries, while being 100% waste-free along the whole manufacturing chain. We have successfully prepared a hard magnet from recycled magnetic materials. The rare earths are on the top of the list of CRMs (critical raw materials), so the recycling of Nd-Fe-B magnets is one of the top European priorities.

This is also one of the important research topics of the DEMETER Marie-Curie European Training Network. Our research is focused on utilizing a contemporary technique of spark plasma sintering (SPS), offering a minimized grain coarsening for the restoration and improvement of the magnetic performance. SPS experiments have demonstrated an improvement of coercivity of the raw HDDR (hydrogenation-disproportionation-desorption-recombination) powder to  $H_c = 1120$  kA/m in a sintered magnet. A post-sinter annealing even resulted in an enhanced  $H_c = 1190$  kA/m, most possibly due to the redistribution of the grain boundary Nd-rich phase. The synthesis part of the work was significantly supported by transmission electron microscopy **studies of interfaces in reprocessed HDDR Nd-Fe-B permanent magnets**. We developed a special Protective Atmosphere Transfer System, which enables advanced micro- and nano-characterization without exposing samples to oxidation. In the frame of DEMETER we also cover the fields of the development of novel hard magnetic  $NdFe_{12}N_x$ -based magnets by electrodeposition. Recent experiments were performed in ionic-liquid-based 1-Ethyl-3-methylimidazolium dicyanamide ([EMIM][DCA]) electrolytes in a protective atmosphere. Nd-Fe-based microns-thick films were successfully deposited with the composition close to the desired  $NdFe_{12}$  ratio. The EDS spectra did not show a significant oxygen content, which shows that these films have the potential to be used as novel permanent magnets.

## Complex Intermetallic Alloys.

In the frame of the **International Associated Laboratory (LIA) PACS2** in which the main goal is to improve our understanding of the mechanisms that promote complexity in metallic alloys, we studied the magnetic structure of a single crystal of the composition  $Cu_{84}Gd_9Ca_7$  (at.%), which was grown by Czochralski pulling from the melt. Although Ca and Gd do not mix in the binary phase diagram, we could find on which atomic sites Gd and Ca are randomly distributed and completely determine the crystal structure. The low-temperature random anisotropy of the ferromagnetic structure was pointed out and its lock-in behaviour below a critical temperature of 24K was studied. We placed quite some effort on studying the crystallization path of a glass prepared by melt-spinning the well-known  $Al_{62}Cu_{25}Fe_{13}$  alloy, which leads to a stable quasicrystal, but replacing Al by another trivalent element such as Ce or Gd. The rare earth kills the aperiodic order at low concentrations, but favours glass formation to such an extent that we could prepare bulk amorphous samples by pulsed electric current sintering of melt-spun ribbons. The crystallization products of these samples were identified and the reaction kinetics is under study. The Al-Cr-Sc system looks very promising so far. For the first time, we discovered a ternary compound in this system, which is still under investigation. It is reminiscent of the  $\gamma$ -brass phase known in the Al-Cr and derived systems. Superstructures with large lattice parameters were also pointed out. Complex lattice defects are observed and delight the electron



Head:

**Prof. Spomenka Kobe**



microscopy experts attached to the LIA. Finally, we dedicated a substantial amount of work to publish our results as well as those obtained by companion groups at the Faculty of Metallurgy and the Institute of Chemistry, respectively. The first stream of results ends up in the possibility to develop a new family of light alloys that will compete with alloys containing CRMs such as Mg. The second stream of work evidences the catalytic performance for the formation of water of the  $\text{Cu}_5(\text{Ca},\text{Gd})$  alloy (already mentioned) just above room temperature in the presence of a mixture of  $\text{H}_2$  and  $\text{O}_2$ . More work is required to fully interpret this data.

#### Structural Materials.

For more than 10 years fusion has been one of our important research activities. To achieve high efficiency and safe operation of the future fusion power plants, large efforts are related to the selection and optimization of suitable structural materials capable of withstanding extreme conditions. One of the key problems is the selection of materials for the divertor, which is responsible for power exhaust and impurity removal via guided plasma exhaust and is therefore subjected to very high heat fluxes. The main task of the High-Heat-Flux Materials (HHFM) division within the EUROfusion program, in which we are a partner, is thus the development of the **components for the DEMO divertor**. Tungsten is considered as a primary candidate for high-heat-loaded structural parts in the DEMO device, mainly due to its very high melting point, good thermal conductivity, low sputtering yield and relatively low activation in terms of long-term waste management. Unfortunately, these advantages are accompanied by a low fracture toughness in the lower-temperature regime, and the onset of recrystallization resulting in a loss of strength at high temperatures that severely limits the operating temperature window. We are trying to overcome the disadvantages of pure W by the incorporation of SiC fibres (to increase the fracture toughness) and/or  $\text{W}_2\text{C}$  nanoparticles (to prevent the recrystallization and grain growth of W) into the W matrix. So far we have determined the most suitable carbon precursor and amount of it for the *in-situ* synthesis of  $\text{W}_2\text{C}$  nanoparticles. Furthermore, we have also optimized the sintering conditions for **W- $\text{W}_2\text{C}$  composites**. Additionally, we have shown that the incorporation of  $\text{W}_2\text{C}$  nanoparticles prevents the W-grain growth, even at temperatures higher than 1000 °C (operating temperature).

#### Materials for Health and Clean Environment.

Part of the research of the department is focused on **bio materials**. In the frame of the COST Action NEWGEN (“New generation biomimetic and customized implants for bone engineering”) we continued with the synthesis and physical and biological characterization of fibroin composite scaffolds for the treatment of osteochondral

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**A national project on magnetooptically coupled nanomaterials for innovative cancer treatments continued with in-vitro studies of biofunctionalized FePt/SiO<sub>2</sub>/Au nanoparticles (NPs) on three cell lines: normal porcine urothelial cells (NPU), low-grade (RT4) and high-grade (T24) cancer urothelial cells in collaboration with the Institute for Cell Biology, University of Ljubljana. After photothermal treatment, a drop in cell viability by 50 % was observed, which is in accordance to the NPs uptake of the RT4 and T24 cell lines, which was 15 and 13 %, respectively. The hybrid FePt/SiO<sub>2</sub>/Au NPs, which we have developed produce a significant photothermal effect and can be effectively used on cancerous cells (Figure 1).**

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defects. Using HRTEM analysis we were able to explain how the  $\text{Ca}^{2+}$  ions that are released from the bioactive glass can change the protein secondary structure, mainly the size of beta-sheets domains, that effectively control the scaffold's properties (in collaboration with the Biochemistry Department B2 and the Veterinary Faculty). In collaboration with Animacel d.o.o. we have expanded the knowledge of fibroin to the synthesis of films and patches for the treatment of large skin wounds in animals. Different surface modifications of fibroin films by conjugation with biological molecules were tested and their biological responses were compared. Several films were already used in the **experimental stem-cell treatment** of large skin/underskin wounds on dogs.

In collaboration with Belgrade University, new methods for the production of graded and biphasic scaffolds based on GG (gellan gummi) and BAG (bioactive glass) were utilized and optimized. The obtained results confirmed the possibility to produce scaffolds by the electrophoretic deposition (EPD) technique based on GG with a graded concentration of BAG aimed at osteochondral tissue engineering.

3D printing was investigated for the printing of various scaffolds (Figure 2). Thermosensitive bio-inks based on gellan gum, fibroin and calcium were developed, measuring the rheological properties of ink composites. We also started with the development of a powder-bed 3D printer for printing inorganic scaffolds, i.e., hydroxyapatite.

Within the Era Chair ISOFood project, a colorimetric assay for  $\text{TiO}_2$  nanoparticle detection in complex matrices of food samples was developed. An established colorimetric method was adopted for the specific detection of the presence of nanosized  $\text{TiO}_2$ . The influence of surfactants, titania crystallinity and buffer medium on the accuracy of spectrophotometric detection was evaluated.

We analysed the physical and chemical properties of different industrial and commercially used nanoparticles in the frame of the project “Evaluation of possible harmful effects of nanoparticles and underlying mechanisms – from

physio-chemical and *in vitro* toxicity characterization to innate immune system activation". The main focus was on the colloidal properties in different cell media and on the solubility of possible harmful ions from the particles under physiological conditions. The results obtained in a collaboration with the Faculty of Electrical Engineering will help us to understand the response of cells to specific materials.

In the field of **dental ceramics** we are addressing major issues concerning the production of zirconia (3Y-TZP) dental restorations, their cementation and behaviour in clinical conditions (*in vivo*) in close cooperation with the Department of Prosthetic Dentistry, Medical Faculty, University of Ljubljana. An extensive study was published in *Dental Materials* on the complexity of the relationships between the sandblasting, ageing and strength of 3Y-TZP with different grain sizes and therefore different transformability. It was shown that fine-grained ceramic exhibited superior degradation resistance, while the coarse-grained ceramic experienced higher surface strengthening and a substantially improved ageing resistance upon sandblasting.

In the framework of the **Climate-KIC Accelerator programme**, which we have been part of, we have successfully met with a few companies that are spending a substantial amount of money for the treatment of their wastewater and need a highly efficient solution to reduce their treatment costs. An analysis of our device for the purification of their wastewater is planned after testing the new device's efficiency for the degradation of model organic substances such as caffeine and phenol, which we have already successfully mineralized in the past.

In the field of sensing and with the foreseen environmental application, we have developed Ni-based receptor elements for sensing different organic analytes using formaldehyde as an example. The modified Ni (Ni-OOH) electrode displays a remarked electro-catalytic activity for the oxidation of HCHO and exhibits a linear relationship in a wide concentration range with LOD 0.001 M. These advantages of porous Ni film make it promising for providing a low cost and **simple sensing method in real environments**.

In the last year we also studied the **fabrication and design of functionalised coatings** on metals. Such coating is attractive because of the wide range of applications and consequently the large impact, which such materials potentially have. We evaluated the possibilities of hydro- and solvothermal treatment along with simple post-processing methods on metallic aluminium and zinc to obtain **new materials** with novel or improved properties, such as self-cleaning, superhydrophilicity, superhydrophobicity, photocatalytic degradation of organics and dielectric properties. These improved properties were achieved by the formation of nano- and micro-sized coatings of titanium dioxide (TiO<sub>2</sub>), zinc oxide (ZnO) and aluminium oxide hydroxide - boehmite ( $\gamma$ -AlO(OH)).

#### Engineering and Functional Ceramics.

In collaboration with the Materials Science Institute of Madrid, we have developed cellulose nanofibre-reinforced engineering electro-conductive ceramics and filed a Great Britain patent application. Imparting electrical conductivity to a dielectric ceramic like alumina or zirconia with conducting nanocarbons (nanotubes or graphene) is challenging due to colloidal instability, particle segregation resulting in inhomogeneity. Instead, we used a small addition of cellulose nanofibres, which render highly homogeneous ceramic dispersions due to the increased hydrophilicity character. Nanofibres not only significantly reinforce the ceramic green body, but upon sintering also convert to finely distribute graphitic ex-cellulose carbon nanofibres within a dense and refined ceramic matrix, resulting in highly electro-conducting alumina and zirconia ceramics.

**Translucent, self-reinforced mullite ceramic** was developed by SPS sintering. Small amounts of yttria and silica in combination with SPS sintering provided enhanced densification, also provoking anisotropic grain growth at low sintering temperatures and pressures. Thus, it was possible to meet the conflicting demands for obtaining a dense mullite with anisotropic grains, ensuring good mechanical properties, while preserving a high light transmittance. The results were published in the *Journal of the American Ceramic Society* and received a best poster award

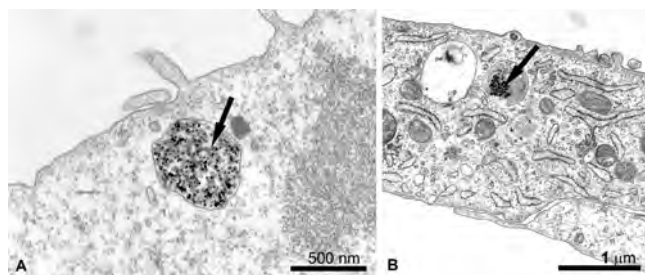


Figure 1: Internalization of hybrid NPs into high-grade cancer urothelial cells *in vitro* (A and B). (Courtesy of Mateja Erdani Kreft and Samo Hudoklin, Institute for Cell Biology, Medical Faculty, University of Ljubljana)



Figure 2: 3D printed gellan gum hydrogel

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**In the field of photocatalysis we have developed a new, innovative device for efficient water and air purification at relatively high flow rates. The main part of the device is a photocatalytically active material, which we synthesized using an anodic oxidation process. For the purpose of making a bigger device, we have developed a process that enables the simple synthesis of the photocatalytically active titania nanotubes that are rigidly attached to a specially shaped metal titanium foil used in our device.**

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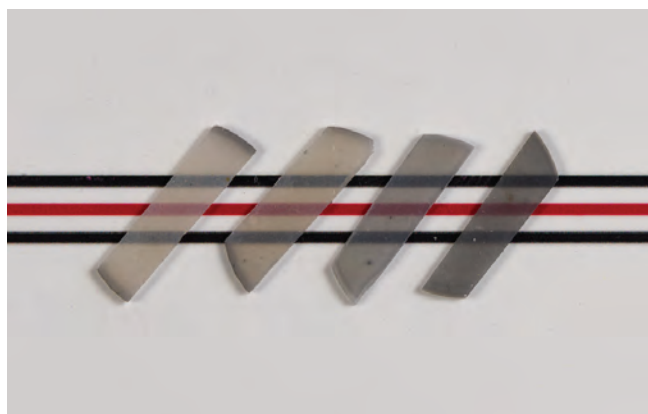


Figure 3: Translucent mullite ceramics.

among 129 competitors at the 41<sup>st</sup> International Conference and Expo on Advanced Ceramics and Composites, in Daytona Beach, Florida (Figure 3).

In the field of **thermoelectrics**, we studied the nanostructure and thermoelectric properties of an n-type thermoelectric material based on  $\text{Sr}(\text{Ti},\text{Nb})\text{O}_3$  that has a perovskite structure. The addition of SrO and CaO into this structure caused the formation of a three-dimensional network of Rudlesden-Popper-type planar faults within the material. The random stacking of planar faults increased the phonon scattering and lowered the thermal conductivity. Consequently, the material exhibited an increased figure of merit ZT. The influence of the synthesis parameters on the microstructure development and consequently the thermoelectric characteristics was also studied in a p-type  $\text{Ca}_3\text{Co}_4\text{O}_9$  ceramics and n-type ceramics of  $\text{Zn}_k\text{In}_2\text{O}_{k+3}$  ( $k=5,11,18$ ) homologous phases. The thermoelectric characteristics of the  $\text{Ca}_3\text{Co}_4\text{O}_9$  ceramics were significantly improved by optimizing the microstructural texturing. In the  $\text{ZnO-In}_2\text{O}_3$  system, we determined a mechanism

of the  $\text{Zn}_k\text{In}_2\text{O}_{k+3}$  homologous phase formation and explained its influence on the microstructure development and consequently thermoelectric characteristics of ceramics.

The influence of the hydrothermal synthesis process on the development of ZnO crystals with a specific morphology was studied. We associated the diverse morphology of the precipitated crystals to the differences in the transient crystallization processes during the precipitation. By altering the pH of the suspension after the precipitation, we gain control over the morphology of the ZnO and show how to grow identical crystallites with different shapes and crystal sizes. We were the first to find how ZnO platelets grow in a certain  $\text{Zn}^{2+}/\text{OH}^-$  ratio along the basal and one of the prismatic directions to form **spherulites** with a very high surface area. We also explained how sphere-like hierarchical structures composed of plate- or rod-like ZnO crystals form through self-assembly driven processes. The research on the hydrothermal synthesis of the **transparent conductive ZnO films** was focused on the influence of the Al-doping on growth, microstructure and optical properties of the ZnO films. The applications are foreseen in LC displays, touch screens and photovoltaic panels.

Within the frame of collaboration with the research group from Sabanci University, Istanbul, Turkey, we successfully realized several studies related to structure-property relationships of **functional oxide ceramics**. One

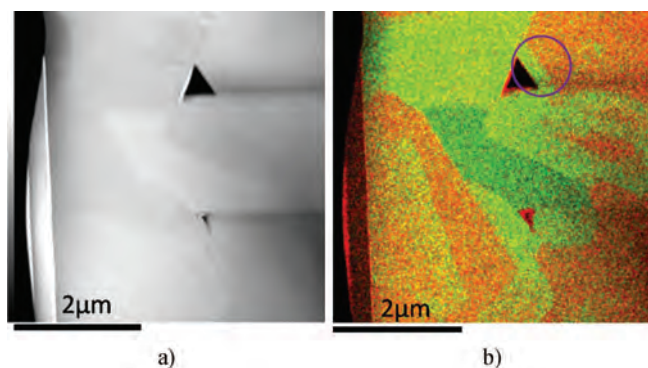


Figure 4: Flash sintering experiments, a) STEM-ADF image, b) STEM-EDX colour maps: K and Na ion atom distribution (K: green, Na: red).

is related to the development of long persistence phosphors as promising materials for energy-saving applications, due to their ability to temporarily store and release light. We confirmed that boron dramatically extends the afterglow persistence to longer than 8 h in strontium aluminates. A second study is related to flash sintering experiments that were for the first time performed on sodium potassium niobate (KNN) ceramics. A theoretical density of 94% was achieved in 30 s under a 250 V/cm electric field at 990°C. These conditions are around 100°C lower and faster than the conventional sintering conditions. Detailed microstructural and chemical investigations of the sample showed that there was inhomogeneous Na, K distribution, resembling a coreshell structure where K is more in the shell and Na is more in the core region (Figure 4). Our latest study deals with the structural and electronic modifications on  $\text{TiO}_2$  anatase by Li, K or Nb doping below and above the solubility limit. XRD results have shown that the anatase-to-rutile

phase transition as a function of temperature was suppressed by potassium and niobium incorporation, whereas it was facilitated by lithium incorporation.

The theoretical part of our research encompassed the density-functional theory to investigate the influence of the substrate on the potentially technologically interesting properties of the **borophene- a single atomic layer of boron atoms**, similar to graphene.

#### Minerals.

Part of the activities of the Department for Nanostructured Materials is focused on minerals as natural heritage. These basic studies help us to understand and use the knowledge in tailoring new materials. In the area of **twinning, epitaxies and phase transformations in minerals** we studied twinning in **pyrite** ( $\text{FeS}_2$ ) from the Mt. Katarina locality near Ljubljana, where interpenetration pyrite twins occur in addition to single pyrite crystals. Analyses of twin boundaries and inclusions in pyrite crystals with techniques of high-resolution transmission electron microscopy showed that remnants of mineralizing fluids entrapped at the interfaces between the inclusions and hosting pyrite contain trace amounts of Pb and Cu, indicating their presence in the surrounding solutions throughout the

pyrite crystallization period. The atomic-scale analysis of the twin boundaries revealed that the formation of the interpenetrating twins is a consequence of complex 3D intergrowths of primary {110} twins enriched in Cu and secondary interfaces along {100} planes which are chemically unchanged. The results indicate that the formation of twins in pyrite is in accordance with the chemically induced twinning mechanism.

We have explained the mechanism of self-assembling of rutile mesocrystals under hydrothermal synthesis conditions leading to the formation of hierarchical nanostructures which exhibit superior efficiency in photo-electrochemical production of hydrogen and **improved solar-energy conversion efficiency**. We have shown that complex branched structures form as a result of the oriented assembly of precipitated fibres along {110} and {101} planes, resulting in lateral attachment and twinning. As precipitates are thermally agitated, their electromagnetic fields are coupled, and nanocrystals are aligned parallel to their longer axis. Due to a multiplicity of interactions, the particles are first attracted into a loosely associated arrangement. However, as the distance between the fibres becomes shorter the crystallographic alignment along the lowest energy planes becomes dominant. Our pioneering study was the first to clearly indicate the presence of electromagnetic force fields that convey critical structural information through which the oriented attachment of nanocrystals is accomplished. The results are published in the prestigious "Scientific Reports". In collaboration with our colleagues from Novosibirsk we studied the conditions that lead to the perfect splicing of beryl seeds into one larger single crystal under hydrothermal conditions. In our group we characterized the contact region between the intergrown crystals down to the atomic scale. We found that the presence of Si-rich amorphous pockets at the interface compensates for the small angular misfit between the oppositely growing domains (Figure 5).

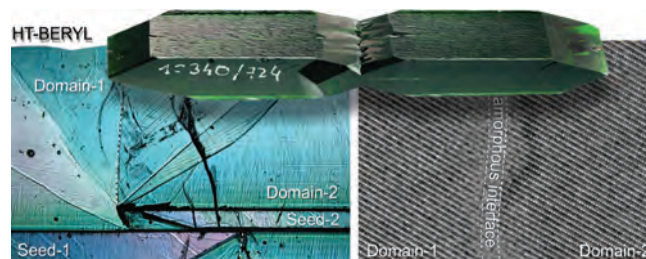


Figure 5: The possibility of the intergrowth of two bulk crystals to a single crystal was demonstrated on the example of beryl, growing under hydrothermal conditions.

#### Analytical Electron Microscopy

For the microstructural characterization of modern materials, we have applied advanced high-resolution scanning electron microscopy (FEGSEM) and analytical methods of energy-dispersive and wavelength-dispersive spectroscopy (EDS, WDS) for qualitative and quantitative elemental analysis. With the implementation of the method of electron backscatter diffraction (EBSD) we have investigated crystallographic characteristics of the materials: crystallinity, orientation of phases and texture.

The FEGSEM, EDS, WDS and EBSD methods were modified and optimized taking into account the specificity of individual materials with the aim to achieve the most precise and accurate analytical results. We investigated a variety of innovative materials such as ceramic thermoelectrics, complex metallic alloys and quasicrystalline alloys, magnetic materials, abrasives, and phosphorescent ceramics.

Using the EBSD analysis we have confirmed the presence and determined the type of twins in thermoelectrics based on polycrystalline  $\text{SnO}_2$ . We investigated the effects of heat treatment on the microstructure and phase composition of complex metallic alloys formed in Al-Cr-Sc materials. With advanced quantitative WDS analysis we have accurately determined small concentrations of rare-earth dopants Dy and Eu in phosphorescent ceramics based on  $\text{Sr}_4\text{Al}_{14}\text{O}_{25}$ .

We successfully finished the **ESTEEM2 project**, which was the only EU project dealing with methodology in **electron microscopy** analytical techniques. In view of this, we have successfully implemented electron microscopy techniques such as electron energy-loss spectroscopy (EELS), high-resolution scanning transmission electron microscopy (STEM, HAADF-STEM), electron holography and mechanical preparation of the TEM samples. Implementation of various electron microscopy analytical techniques and the possibility for the researchers to access research infrastructure for electron microscopy within the **Center for Electron Microscopy and Microanalysis (CEMM)** is of utmost importance for the research group.

#### Industrial partners.

We have provided high-temperature laboratory ceramics to Lithoz GmbH Vienna, Hidria Rotomatika Spodnja Idrija, ESAL d.o.o., and Brno University of Technology, Brno. We have collaborated with many partners from

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**The main part of our research within the frame of Liquid TEM studies was focused on the nucleation and early growth of  $\text{TiO}_2$  and yttrium-based nanoparticles using the liquid cell inside of a transmission electron microscope (TEM). During heating of the solution to elevated temperatures we were able to record high-frame-rate videos of dynamic changes in electron diffraction patterns during the entire nucleation and growth process of the crystals, enabling us to later exactly reconstruct crystallographic changes during the whole process (Figure 6).**

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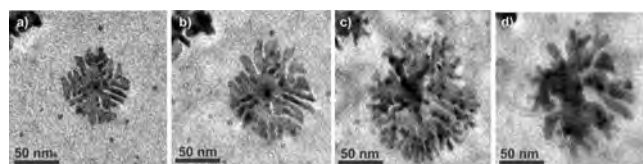


Figure 6: Growth sequence of dendritic nanoparticles in solution observed under dynamic conditions using the liquid TEM method (a-c).

industry and other research institutions by performing the analyses of specific materials. Main collaborations were with Domel Železniki, Akrapovič Ivančna Gorica, Ustna Medicina Ljubljana, Silkem Kidričevo and Errantech Hangzhou. For SwatyComet, we have conducted analyses of innovative composite abrasives within the project "Microstructural investigations of abrasive materials", which are intended to develop and manufacture improved cutting and grinding tools with a significantly prolonged lifetime. For RC eNeM we were developing microvaristor powder for composites with nonlinear resistivity.

#### Education and outreach activities.

The members of the Department are heavily involved in the educational system in Slovenia and abroad. Especially, our members dedicate themselves to the educational process of the Jožef Stefan International Postgraduate School, FKKT, NTF, and FMF.

In the frame of the project **Science on the street** (Znanost na cesti - ZnC) founded and coordinated by the members of the department, we are closely involved in raising public awareness in the promotion of science. For the last 4 years, the project activities were performed under the patronage of SATENA (the Slovenian Scientific–Technological Association). In the last year, we organized two cycles of popular scientific talks, scientific slam, round table, and we published several scientific blogs. We organized the scientific competitions for young scientists and students.

#### Awards and appointments

1. **Luka Suhadolnik**, 3<sup>rd</sup> Best Oral Presentation at the 24<sup>th</sup> International Conference on Materials and Technology, Portorož, Slovenia, 28-30 September 2016. Title of the awarded contribution: Optimization of Photoelectrocatalytic Activity of TiO<sub>2</sub>-based Microreactor (co-authors: Andrej Pohar, Blaž Likozar and Miran Čeh)
2. **Ana Gantar**, Nataša Drnovšek, Rok Kocen, Saša Novak, Special prize for Innovations for Economy for "SilkPatch - Innovative Solution for Chronic Skin Wounds", 9<sup>th</sup> International Technology Transfer Conference & Innovation Day 2016, Brdo pri Kranju, 21 September 2016
3. **Nina Kostevšek**, Best Young Lecturer Award, 2nd International Symposium on Nanoparticles-Nanomaterials and Applications (ISN2A-2016), Lisbon, Portugal, 8-21 January 2016. Title of the awarded contribution: "Multimodal hybrid FePt/SiO<sub>2</sub>/Au nanoparticles for nanomedical applications: New synthesis approach for improved magnetic and optical properties" (co-authors: Sašo Šturm, Igor Serša, Ana Sepe, Matjaž Spreitzer, Spomenka Kobe, Kristina Žužek Rožman)

#### Organization of conferences, congresses and meetings

1. Symposium: Design and Recycling of Rare-Earth (RE) Permanent Magnet (PM) Motors and Generators in Hybrid and Full Electric Vehicles – DEMETER, Ljubljana, 14 March 2016
2. EMAS 2016 - 12<sup>th</sup> Regional Workshop on Electron Probe Microanalysis of Materials Today - Practical Aspects, Bagnols-sur-Cèze, France, 8–11 May 2016 (members of European Microbeam Analysis Society Board)
3. 24<sup>th</sup> International Conference on Materials and Technology – 24 ICM&T, 28–30 September, Portorož (co-organisers)
4. C-MAC Days 2016, Bratislava, Slovakia, 21–23 November 2016 (members of Science Board and General Assembly in European Integrated Center for the Development of New Metallic Alloys and Compounds (C-MAC))

#### Patent granted

1. Luka Suhadolnik, Matic Krivec, Miran Čeh, Kristina Žagar, Goran Dražič, Photocatalytic reactor, SI24802 (A), Slovenian Intellectual Property Office, 31. 03. 2016

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## INTERNATIONAL PROJECTS

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| <ol style="list-style-type: none"> <li>1. Selective Laser Melting (SLM) and Spark Plasma Sintering (SPS) of Cost Effective Rare-earth based Permanent Magnets for Electrical Machines<br/>Prof. Spomenka Kobe<br/>Abb Switzerland Ltd</li> <li>2. PurBox - Prototype of the Photoelectrocatalytic Reactor<br/>Luka Suhadolnik, B. Sc.<br/>Provdavis School Of International</li> <li>3. 7FP - ESTEEM 2; Enabling Science and Technology through European Electron Microscopy<br/>Prof. Miran Čeh<br/>European Commission</li> <li>4. 7FP - MAG-DRIVE; New Permanent Magnets for Electric-Vehicle Drive Application<br/>Asst. Prof. Matej Andrej Komelj<br/>European Commission</li> <li>5. 7 FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety</li> </ol> | <p>and Traceability<br/>Prof. Saša Novak Krmpotič<br/>European Commission</p> <ol style="list-style-type: none"> <li>6. COST MP1301 NEWGEN; New Generation Biomimetic and Customized Implants for Bone Engineering<br/>Prof. Saša Novak Krmpotič<br/>Cost Office</li> <li>7. COST ES1205; The Transfer of Engineered Nanomaterials from Wastewater Treatment &amp; Stormwater to Rivers<br/>Prof. Saša Novak Krmpotič<br/>Cost Office</li> <li>8. H2020 - REProMag; Resource Efficient Production Route for Rare Earth Magnets<br/>Dr. Benjamin Podmiljšak<br/>European Commission</li> <li>9. H2020 - DEMETER; Training Network for the Design and Recycling of Rare-Earth Permanent Magnet Motors and Generators in Hybrid and Full Electric Vehicles<br/>Asst. Prof. Kristina Žužek Rožman<br/>European Commission</li> </ol> |
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10. H2020, EUROFUSION; Materials-PPPT-FU: WC and SiC Reinforced Tungsten  
Prof. Saša Novak Krmpotič  
European Commission
11. H2020, Education-ED-FU, EUROFUSION  
Prof. Saša Novak Krmpotič  
European Commission
12. Advanced Methods and Technologies for Processing of a New Generation of ZnO-based Varistor Ceramics  
Prof. Slavko Bernik  
Chinese Academy of Sciences, Shanghai
13. Irradiation and Analysis of Nano SiC Samples  
Dr. Aljaž Iveković  
National Nuclear Research Center, Azerbaijan
14. Determination of Minority Phases, Quantitative Analysis and Determination of Lattice Parameters in SPS Sintered Samples Analysis and Determination of Lattice Parameters in SPS Sintered Samples  
Dr. Petra Jenuš Brdnik  
Jecs Trust
15. Electron Microscopy Study of the Degradation Kinetics of Porous Bioactive Glass based Novel Drug Eluting Implants (Coating/3D Scaffolds) as a Function of Hard Tissue Regeneration for Treatment of Osteoporotic Fractures in Elderly Patients  
Asst. Prof. Nina Daneu  
BI-IN/15-17-015  
Slovenian Research Agency
16. Nucleation and Photocatalytic Activity of Nanoparticles Studied in Actual Liquid Environment under Transmission Electron Microscope  
Prof. Sašo Šturm  
Slovenian Research Agency  
BI-JP/15-17-001
17. Atomic-scale Studies of Topotaxial Reactions in Minerals with the Rutile and Corundum-type Structures  
Asst. Prof. Nina Daneu  
Slovenian Research Agency  
BI-US/15-16-065
18. 0D to 3D ZnO Nanostructures for Optical, Electronic and Energy Applications  
Dr. Matejka Podlogar  
Slovenian Research Agency  
BI-RS/16-17-053
19. Synthesis of Core/Shell MgAl<sub>2</sub>O<sub>4</sub> Spinel Powders for Transparent Armor and IR Applications – CSMASP  
Prof. Slavko Bernik  
Slovenian Research Agency  
BI-TR/16-18-003
20. Processing of High-performance Zirconia Bioceramics for Dental Application  
Asst. Prof. Andraž Kocjan  
Slovenian Research Agency  
BI-HR/16-17-035
21. Investigations of Twinning and Topotaxial Reactions in Sulphide Minerals  
Prof. Aleksander Rečnik  
Slovenian Research Agency  
BI-HR/16-17-029
22. Crystal and Electronic Structure of NbS<sub>3</sub> Phases  
Prof. Sašo Šturm  
Slovenian Research Agency  
BI-RU/16-18-048
23. Crystallography, Twinning and Phase Transformations in Minerals with Aragonite-Type Structure (CaCO<sub>3</sub>, SrCO<sub>3</sub>, BaCO<sub>3</sub>, PbCO<sub>3</sub>)  
Prof. Aleksander Rečnik  
Slovenian Research Agency  
BI-RU/16-18-004
24. Structural and Microstructural Engineering of ZnO Thermoelectrics (SMEZ)  
Prof. Slavko Bernik  
Slovenian Research Agency  
BI-FR/15-16-PROTEUS-007

## RESEARCH PROGRAMS

1. Engineering and bio-ceramics  
Asst. Prof. Andraž Kocjan
2. Nanostructured Materials  
Prof. Spomenka Kobe

## R & D GRANTS AND CONTRACTS

1. Atomic-scale studies of initial stages of phase transformations in minerals  
Asst. Prof. Nina Daneu
2. Structure and Chemical Composition Study of Surfaces and Interfaces with High-resolution Scanning Transmission Electron Microscopy at Atomic Level  
Prof. Aleksander Rečnik
3. Bio-responsive magneto-optically coupled nanomaterial-based systems for innovative skin cancer treatments  
Prof. Sašo Šturm
4. High-Performance Nanostructured Coatings - breakthrough in concentrated solar power  
Asst. Prof. Andraž Kocjan
5. From the synthesis of metal oxides to the humidity and oxygen prototype nanosensors  
Dr. Kristina Žagar Soderžnik
6. High-coercivity Nd-Fe-B permanent magnets with minimum amount of heavy rare earths  
Dr. Marko Soderžnik

## NEW CONTRACTS

1. Preparation of microvaristor powder for composites with nonlinear resistivity  
Prof. Slavko Bernik  
Razvojni Center eNeM Novi Materiali d. o. o.
2. Research & development of dental materials  
Dr. Nataša Drnovšek, Asst. Prof. Andraž Kocjan  
Ustna medicina, d.o.o.
3. Microstructural investigations of abrasive materials  
Dr. Zoran Samardžija  
SwatyComet, d.o.o.

## VISITORS FROM ABROAD

1. Dr. Cristina Echevarria-Bonet, Institute for Energy Technology (IFE), Physics Department, Kjeller, Norway, 30 January – 7 February 2016
2. Nerea Gonzales, Marta Navarro, Universidad Rey Juan Carlos, Madrid, Spain, 16 February – 14 May 2016
3. Prof. Mihály Pósfai, University of Pannonia, Veszprém, Hungary, 18–22 February 2016
4. Prof. István Dódy, dr. Ildikó Cora, Erzsébet Dodony, Eötvös Loránd University, Budapest, Hungary, 18 – 22 February 2016
5. Dr. Milivoj Plodinec, Ruder Bošković Institute, Zagreb, Croatia, 25–27 February 2016
6. Prof. Cleva Ow Yang, Sabanci University, Istanbul, Turkey, 6–10 March 2016
7. Dr. Milivoj Plodinec, Dr. Irena Kereković, Ruder Bošković Institute, Zagreb, Croatia, 14–26 March 2016
8. Dr. Julian Ledieu, Joris Kadok, Institut Jean Lamour, Nancy, France, 25–29 March 2016
9. Prof. Kazuhiro Hono, National Institute for Materials Science (NIMS), Tsukuba, Japan, 7–9 May 2016
10. Dr. Elinor Grace Castle, Queen Mary University of London – QMUL, London, United Kingdom, 13 May – 4 June 2016
11. Dr. Goran Štefanić, Ruder Bošković Institute, Zagreb, Croatia, 17–18 May 2016
12. Dr. Magnus H. Sorby, Institute for Energy Technology, Physics Department, Kjeller, Norway, 25–28 May 2016
13. Dr. Richard Wheeler, Edinburgh Scientific, Edinburgh, Scotland, 28 May – 1 June 2016
14. Dr. Goran Branković, Marina Vuković, Vesna Ribić, Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia, 1–8 June 2016
15. Dr. Bernd Wicklein, Instituto de Ciencia de Materiales de Madrid – ICMM, Madrid, Spain, 13–24 June 2016
16. Dr. Émilie Gaudry, Institut Jean Lamour, Nancy, France, 8–15 July 2016
17. Fabian Burkhardt, University of Applied Sciences Aalen, Engelsbrand, Germany, 1 August 2016 – 28 January 2017
18. Dr. Mauro Alini, AO Foundation, Davos, Switzerland, 24–25 August 2016
19. Dr. Yuki Kimura, Dr. Jun Kawano, Tomoya Yamazaki, University of Hokaido, Hokaido, Japan, 24–27 August 2016
20. Dr. Pavel Gavryushkin, Sobolev Institute of Geology and Mineralogy, Novosibirsk, Russia, 2–19 September 2016
21. Prof. Makoto Shiojiri, Kyoto Institute of Technology, Kyoto, Japan, 4–7 September 2016
22. Dr. Richard Wheeler, Edinburgh Scientific, Edinburgh, Scotland, 4–9 September, 2016
23. Matej Baláz, Institute of Geotechnics, Slovak Academy of Sciences, Košice, Slovakia, 10–16 September 2016
24. Dr. Ulrike Wolff, Leibniz-Institut für Festkörper- und Werkstofforschung, Dresden, Germany, 3 October – 31 December 2016
25. Prof. Peter A. van Aken, Stuttgart Center for Electron Microscopy, Max Planck Institute for Solid State Research, Stuttgart, Germany, 11–13 October 2016
26. Sayanthan Ray, Central Glass and Ceramic Research Institute – CSIR, Kolkata, India, 20 October – 20 November 2016
27. Dr. Richard Wheeler, Edinburgh Scientific, Edinburgh, Scotland, 23–28 October 2016
28. Jovana Zvicer, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, 29 October – 4 December 2016

29. Dr. Reinhard Simon, ABB Corporate Research Center, Baden-Dättwil, Switzerland, 9 November 2016
30. Dr. Andrea Čobić, Prof. Vladimir Bermanec, Dr. Snježana Mikulčić Pavlaković, Marin Soufek, M.Sc., Faculty of Science, University of Zagreb, Zagreb, Croatia, 10 November 2016
31. Vesna Ribić, Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia, 16 November – 16 December 2016
32. Dr. Goran Branković, Marina Vuković, Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia, 16–23 November 2016
33. Prof. Mehmet Ali Gülgün, Sabanci University, Istanbul, Turkey, 23–25 November 2016
34. Dr. Andrea Čobić, Dr. Snježana Mikulčić Pavlaković, Faculty of Science, University of Zagreb, Zagreb, Croatia, 24–29 November 2016
35. Prof. Emmanuel Guilmeau, Cédric Bourges, Laboratoire CRISMAT, Caen, France, 28 – 30 November 2016
36. Asst. Prof. İsmail Özgür Özer, Anadolu University, Department of Materials Science and Engineering, Eskişehir, Turkey, 7–11 December 2016
37. Dr. Julian Ledieu, Dr. Vincent Fournée, Dr. Marie-Cécile de Weerd, Institut Jean Lamour, Nancy, France, 12–15 December 2016

## STAFF

### Researchers

1. Prof. Slavko Bernik
2. Prof. Miran Čeh
3. Asst. Prof. Nina Daneu
4. Prof. Jean Marie Dubois
5. **Prof. Spomenka Kobe, Head**
6. Asst. Prof. Andraž Kocjan
7. Asst. Prof. Matej Andrej Komelj
8. Prof. Saša Novak Krmptič
9. Dr. Benjamin Podmiljšak
10. Prof. Aleksander Rečnik
11. Dr. Zoran Samardžija
12. Prof. Sašo Šturm
13. Dr. Kristina Žagar Soderžnik
14. Asst. Prof. Kristina Žužek Rožman

### Postdoctoral associates

15. Dr. Nataša Drnovšek
  16. Dr. Ana Gantar
  17. *Dr. Aljaž Iveković, on leave 01.03.16*
  18. Dr. Petra Jenuš Brdnic
  19. *Dr. Martina Lorenzetti, left 21.12.16*
  20. *Dr. Darja Pečko, left 01.03.16*
  21. Dr. Matejka Podlogar
  22. Dr. Marko Soderžnik
- ### Postgraduates
23. Anže Abram, B. Sc.
  24. Bojan Ambrožič, B. Sc.

25. Sandra Drev, B. Sc.
  26. Hermina Hudelja, B. Sc.
  27. Awais Ikram, B. Sc.
  28. *Dr. Marja Jerič, left 01.11.16*
  29. Vanja Jordan, B. Sc.
  30. Luka Kelhar, B. Sc.
  31. Rok Kocen, B. Sc.
  32. Matej Kocen, B. Sc.
  33. Nina Kostevšek, B. Sc.
  34. *Mateja Košir, B. Sc., left 01.12.16*
  35. Ana Lazar, B. Sc.
  36. Muhammad Farhan Mehmood, B. Sc.
  37. Luka Suhadolnik, B. Sc.
  38. Sara Tominc, B. Sc.
  39. Tomaž Tomše, B. Sc.
  40. Špela Trafela, B. Sc.
  41. Xuan Xu, B. Sc.
- ### Technical officers
42. *Dr. Jana Ferič, left 01.07.16*
  43. Sanja Fidler, B. Sc.
  44. *Martin Topole, B. Sc., left 01.10.16*
- ### Technical and administrative staff
45. Teja Dukić
  46. Darko Eterović
  47. *Mojca Hren, left 21.12.16*
  48. Tomislav Pustotnik

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Somayeh Abdi, Matthias Bönisch, Steffen Oswald, Mohsen Samadi Khoshkhou, Wolfgang Gruner, Martina Lorenzetti, Ulrike Wolff, Mariana Calin, Jürgen Eckert, Annett Gebert, "Thermal oxidation behavior of glass-forming Ti-Zr-(Nb)-Si alloys", *J. mater. res.*, vol. 31, no. 9, pp. 1264-1274, 2016.
2. Anže Abram, Andreja Eršte, Goran Dražić, Vid Bobnar, "Structural and dielectric properties of hydrothermally prepared boehmite coatings on an aluminium foil", *J. mater. sci., Mater. electron.*, vol. 27, no. 10, pp. 10221-10225, 2016.
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4. Muhammad Shahid Arshad, Mariana P. Proenca, Špela Trafela, Volker Neu, Ulrike Wolff, Sven Stienen, Manuel Vazques, Spomenka Kobe, Kristina Žužek Rožman, "The role of the crystal orientation (c-axis) on switching field distribution and the magnetic domain configuration in electrodeposited hcp Co-Pt nanowires", *J. phys., D, Appl. phys.*, vol. 49, no. 18, pp. 1-13, May 2016.
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7. Danielle Cavalcante Guedes de Lima, Tibério Andrade Dos Passos, Marie-Cecile De Weerd, Samuel Kenzari, Rodinei Gomes Medeiros, Severino Jackson Guedes De Lima, Jean-Marie Dubois, "Indirect assessment of the surface energy of the Al-Cu-Fe quasicrystal", *J. Mater. Sci.*, vol. 51, no. 8, pp. 4070-4078, 2016.
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9. Jasna Cotič, Peter Jevnikar, Andraž Kocjan, Tomaž Kosmač, "Complexity of the relationships between the sintering-temperature-dependent grain size, airborne-particle abrasion, ageing and strength of 3Y-TZP ceramics", *Dent Mater*, vol. 32, iss. 4, pp. 510-518, Apr. 2016.
10. Aleš Daksobler, Andraž Kocjan, Paul Bowen, "Predicting the yield stress of paraffin-wax suspensions", *Powder technol.*, vol. 291, pp. 1-6, 2016.
11. Nataša Drnovšek, Rok Kocen, Ana Gantar, Marinka Drobnič-Košorok, Adrijana Leonardi, Igor Križaj, Aleksander Rečnik, Saša Novak, "Size of silk fibroin β-sheet domains affected by Ca<sup>2+</sup>", *J. mater. chem. B*, vol. 4, iss. 40, pp. 6597-6608, 2016.
12. Ana Gantar, Nataša Drnovšek, Pablo Casuso, Adrián Pérez-San Vicente, Javier Rodriguez, Damien Dupin, Saša Novak, Irada Loinaz, "Injectable and self-healing dynamic hydrogel containing bioactive glass nanoparticles as a potential biomaterial for bone regeneration", *RSC advances*, vol. 6, no. 73, pp. 69156-69166, 2016.
13. Petra Jenuš, Martin Topole, Paul J. McGuiness, Cecilia Granados-Miralles, Marian Stingaciu, Mogens Christensen, Spomenka Kobe, Kristina Žužek Rožman, "Ferrite-based exchange-coupled hard-soft magnets fabricated by spark plasma sintering", *J. Am. Ceram. Soc.*, vol. 99, iss. 6, pp. 1927-1934, 2016.

14. Marja Jerič, Johannes de Boor, Boštjan Jančar, Miran Čeh, "An enhanced thermoelectric figure of merit for  $\text{Sr}(\text{Ti}_{0.8}\text{Nb}_{0.2})\text{O}_3$  based on a Ruddlesden-Popper-polytype-induced microstructure", *J. Eur. Ceram. Soc.*, vol. 36, no. 5, pp. 1177-1182, 2016.
15. Marja Jerič, Johannes de Boor, Janez Zavašnik, Miran Čeh, "Lowering the thermal conductivity of  $\text{Sr}(\text{Ti}_{0.8}\text{Nb}_{0.2})\text{O}_3$  by SrO and CaO doping emicrostructure and thermoelectric properties: microstructure and thermoelectric properties", *J. Mater. Sci.*, vol. 51, no. 16, pp. 7660-7668, 2016.
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17. Tjaša Kanduč, Zoran Samardžija, Nataša Mori, Andreja Jerebic, Ines Levčič, Miha Kračun, Johanna A. Robinson, Stojan Žigon, Željko Blažeka, David Kocman, "Hydrogeochemical and isotopic characterization of Pesnica River, Slovenia", *Geologija*, vol. 59, no. 2, pp. 179-192, 2016.
18. Luka Kelhar, Jana Bezjak, Pascal Boulet, Marjeta Maček, Sašo Šturm, Martin Lamut, Boštjan Markoli, Spomenka Kobe, Jean-Marie Dubois, "Stabilisation of Ce-Cu-Fe amorphous alloys by addition of Al", *Philos. mag.* (2003), vol. 96, iss. 30, pp. 3143-3185, 2016.
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20. Andraž Kocjan, Marko Češnovar, Damjan Vengust, Tomaž Kosmač, Aleš Dakskobler, "Translucent yttria- and silica-doped mullite ceramics with anisotropic grains produced by spark plasma sintering", *J. Am. Ceram. Soc.*, vol. 99, iss. 9, pp. 3090-3069, 2016. [COBISS.SI-ID 29511719]
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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 nanoparticles.*

In 2016 our investigations focused on several important materials, i.e., materials containing magnetic nanoparticles, multifunctional nanocomposites, fluorescent nanoparticles, and semiconducting materials for the preparation of thermistors.

The research on nanoparticles-based materials is continuously focused on engineering the nanoparticles' surface properties. Engineering of the 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 interactions between the nanoparticles in a liquid medium. It also significantly determines the interactions of the nanoparticles with biological systems. Research in 2016 was focused on the colloidal stability of nanoparticles dispersed in biological fluids. For reliable biomedical testing any agglomeration of the nanoparticles in different aqueous media at a neutral pH and at an increased ionic strength has to be completely prevented. Moreover, the nanoparticles should not display a large surface charge. Therefore, the suspensions have to be stabilized sterically, with bonding large hydrophilic molecules, e.g., polyethylene glycol (PEG), polysaccharides, or polypeptides, onto the nanoparticle surfaces. The layer of molecules has to be bonded by forming stable covalent bonds, not to be desorbed or exchanged with other ligands from the medium. The surfaces of oxide materials are chemically relatively inert and in general they do not allow covalent bonding of organic molecules. To enable covalent bonding the nanoparticles are coated with a thin silica layer. The silica provides surface silanol -Si-OH functional groups, which enable the covalent bonding of molecules, for example, different silanes. Different strategies for the covalent bonding of PEG, carboxymethyl dextran, and dextran with different molar masses onto the surfaces of different nanoparticles have been tested.

Maintaining the colloidal stability was specially challenging in the case of barium hexaferrite ( $\text{BaFe}_{12}\text{O}_{19}$ ) nanoplatelets, because of their hard-magnetic properties additionally causing agglomeration with magnetic dipole-dipole interactions. The colloidal entirely stable suspensions of such nanoplatelets in a phosphate buffer saline (PBS) were prepared by coating polysaccharide dextran onto the glycidoxypropyl silane (GLYMO) functionalized, silica-coated nanoplatelets. The bonding was enabled with a reaction of epoxy groups of GLYMO at the nanoplatelets' surfaces with hydroxyl groups of dextran. A part of the research was devoted to the synthesis of polypeptide coatings. The polypeptides were synthesized with the covalent crosslinking of amino acids adsorbed on the nanoparticles' surfaces. As we showed in previous research the amino acids adsorb onto the nanoparticles' surfaces in the form of molecular associates in very high surface concentrations, exceeding several tens of molecules per  $\text{nm}^2$ . The associate is formed by binding the amino-acid molecules together with relatively weak hydrogen or electrostatic bonds. As a result, the layer of the adsorbed molecules at the nanoparticle surfaces is very sensitive to different external conditions. To form a stable polypeptide layer two different amino acids, aspartic acid ( $\text{HOOC-CH}_2\text{-CH}(\text{NH}_2)\text{COOH}$ ) and lysine ( $\text{H}_2\text{N}(\text{CH}_2)_4\text{-CH}(\text{NH}_2)\text{COOH}$ ), were adsorbed onto the nanoparticles. The molecules in the adsorbed layer at the nanoparticles' surfaces were then cross-linked with peptide bonds using activation of the carboxyl groups with carbodiimide (EDC) and their reaction with the amino group of the adjacent molecules.

Functionalization of nanoparticles with polypeptides is also the topic of a newly established collaboration with researchers from the University of Trieste. New approaches for the covalent bonding of amino acids and short peptides onto nanoparticles have been developed. Preliminary research was focused on binding hydrophobic amino acids, such as phenylalanine. These kinds of functionalized nanoparticles are suitable for further co-assembly with peptide-based superstructures for the synthesis of functional composite materials. The development of new approaches for the binding of polar amino acids to the magnetic nanoparticles is in progress. It is expected that



Head:

**Prof. Darko Makovec**

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**Immobilization of (bio)catalysts onto superparamagnetic nanoclusters for their magnetic separation.**

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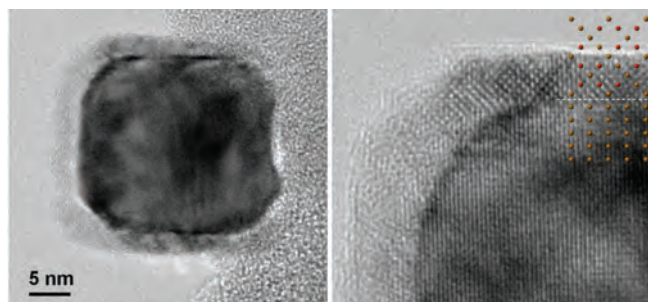


Figure 1: Metal-iron nanoparticles protected with a surface layer of iron oxide magnetite. Magnetite grows epitactically at the iron surface.

functionalization with polar amino acids will enable the colloidal stability of the nanoparticles in biological media.

A large part of the research in 2016 was devoted to the synthesis of metallic iron nanoparticles. The metallic iron displays a saturation magnetization  $M_s$  of over 220 Am<sup>2</sup>/kg. This is much higher than the oxide materials normally used for magnetic nanoparticles. For example, magnetic iron oxide maghemite displays  $M_s$  of approximately 80 Am<sup>2</sup>/kg. However, the problem of the metal nanoparticles (apart from noble metals) is in their very high reactivity, resulting in rapid oxidation when they come into contact with ambient oxygen. To enable handling the iron nanoparticles are usually coated with a layer of crystalline carbon. For the simultaneous synthesis and passivation of the iron nanoparticles, relatively expensive methods based on pyrolysis in the vapour phase are usually applied. We developed an inexpensive method for the synthesis of metal iron nanoparticles based on the heating of specially designed, iron-oxhydroxide nanoparticles in a reducing atmosphere. The nanoparticles very slowly oxidize, resulting in epitactic growth of magnetic iron oxide magnetite (M) on their surfaces ((100)<sub>Fe</sub> || (10-1)<sub>M</sub>, (010)<sub>Fe</sub> || (010)<sub>M</sub>, [001]<sub>Fe</sub> || [101]<sub>M</sub>). The formed oxide surface layer protects the nanoparticle from further oxidation (Figure 1). At an increased temperature in air the passivation is not effective anymore. The nanoparticles oxidize entirely with the diffusion of the Fe atoms through the magnetite surface layer, leaving a void in the nanoparticle's interior. Thus, hollow, rectangular nanoparticles of magnetic iron oxide can be synthesized.

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.

An important part of the research has been devoted to the testing of clusters of superparamagnetic iron-oxide nanoparticles (superparamagnetic nanoclusters) in applications based on magnetic separation.

**A new method for the synthesis of metal-iron nanoparticles was developed. The nanoparticles are protected from rapid oxidation by a surface magnetite layer.**

In magnetic separation the commercially available superparamagnetic nanoclusters produced by Nanos Sci. (<http://nanos-sci.com/>), a spin-out company of the JSI, are normally used. The core of the spherical nanocluster represents an assembly of around 100 nanoparticles. Because of its larger volume the magnetic force acting in a magnetic-field gradient on the nanocluster is much larger than the force acting on the individual superparamagnetic nanoparticle.

The large magnetic force enables the effective magnetic separation of the nanoclusters from the suspension, whereas the individual nanoparticles cannot be separated. The nanoclusters' core is coated with a thin silica shell, which enabled the effective covalent bonding of different functionalization molecules onto their surfaces. The fluorescent molecules are incorporated into the silica shell for tracking of the nanoclusters with methods based on fluorescence microscopy.

A 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 for the 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 nanobiocatalysts. Nanobiocatalysts were tested in multienzymatic synthesis procedures for the stereo-selective synthesis of aminopolyols and iminocyclitols, important in pharmacy and nutraceuticals.

Superparamagnetic nanoclusters are also used as supports for catalysts, such as ruthenium. In collaboration with the National Institute of Chemistry we tested a magnetically separable ruthenium catalyst for chemical reactions of hydrogenation and deoxygenation. Because the previous research showed that the silica shell present at the surfaces of our usual superparamagnetic nanoclusters is not a suitable support for the ruthenium catalyst in the mentioned reactions, we have developed carbon-coated superparamagnetic nanoclusters (Figure 2). The carbon layer on the magnetic nanoparticles was formed by a hydrothermal treatment of the carbohydrates followed by pyrolysis in an inert atmosphere. The temperature of the pyrolysis has a major impact on the amount of graphite, on the amount of oxygen surface groups, and on the amount of defects in the graphite structure. Ru nanoparticles were deposited onto the carbon coating using reduction of a Ru precursor by isopropanol at an elevated temperature. The concentration of the precursor and the temperature of reduction have a major impact on the average size of the Ru nanoparticles. The catalyst exhibited comparable catalytic activity to the commercial one. It can be magnetically

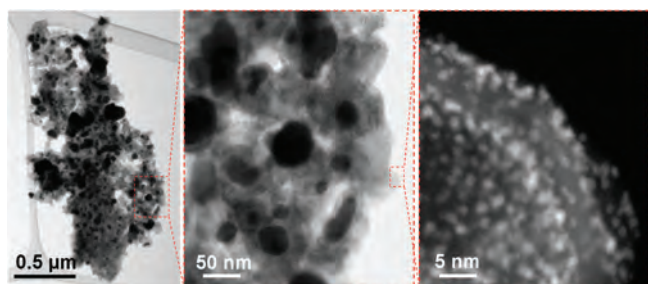


Figure 2: Images of a magnetically retractable catalyst recorded with STEM at increasing magnifications. The catalyst is composed of magnetic particles of metallic iron coated with graphitic carbon, on which small catalytic Ru nanoparticles are deposited (images on the left-hand side and in the middle represent ABF, the image on the right-hand side represents HAADF).

separable nanobiocatalysts. Nanobiocatalysts were tested in multienzymatic synthesis procedures for the stereo-selective synthesis of aminopolyols and iminocyclitols, important in pharmacy and nutraceuticals.

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separated from the reaction mixture after completion of the reaction and even heated by exposure to an alternating magnetic field. In collaboration with the Department for Nanostructured Materials, JSI, a simple procedure for the preparation of superparamagnetic clusters coated with AlOOH and Al<sub>2</sub>O<sub>3</sub> coatings has been developed. Both types of coatings exhibit a large specific surface area. We have successfully prepared Ru(OH)<sub>3</sub> nanoparticles on the surface of the Al<sub>2</sub>O<sub>3</sub> coating. In cooperation with the Faculty of Chemistry and Chemical Technology, University of Ljubljana, the catalysts were tested in oxidations of molecules relevant for pharmacy.

Besides in the magnetic separation, superparamagnetic nanoclusters could also be interesting in many other applications where a 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. Our joint project with researchers from Faculty of Pharmacy, University of Ljubljana, devoted to magnetic drug-delivery systems has been continued. The coating of magnetic nanoclusters with a specially designed porous silica layer allowed the controlled dissolution of one part of iron-oxide nanoparticles from the nanocluster in a strong acid. Thus, a delivery system was developed which retains a sufficient magnetic responsiveness and enables loading and the controlled release of an active pharmaceutical substance through the porous silica shell. A potential anti-cancer drug orlistat was chosen to test the effectiveness of the hollow magnetic nanoclusters. Orlistat is highly hydrophobic and due to its physico-chemical properties very challenging for the preparation of polymeric and lipid-based drug-delivery systems and other pharmaceutical formulations. The remarkable rigidity and robustness of our hollow delivery system enabled loading with orlistat in various solvents. A mixture of ethanol and 1-tetradecanol has been used as a first choice in the on-going research. The tetradecanol displays the solid-to-liquid transformation at temperatures between 38 and 40 °C. Our research efforts were focused on the preparation of a delivery system with controlled drug release. The active substance orlistat was first incorporated into the solid 1-tetradecanol inside the hollow nanoclusters and released once the temperature was increased above a certain value. This thermo-responsive release of the drug at a desired place in the human body can potentially be triggered with heat released during exposure of the remaining magnetic nanoparticles in the hollow nanoclusters to an alternating magnetic field (magnetic hyperthermia).

We continued our research of the magnetic assembly of the superparamagnetic nanoclusters into one-dimensional nanochains in the suspensions. Novel magnetic nanostructures were prepared with magnetic assembly of the nanoclusters coated with silica shells of various thicknesses. First, the nanoclusters with a thin silica shell were assembled into short nanochains. Subsequently, the nanoclusters with a thick silica shell were added to one or both ends of the initial short nanochains under the applied magnetic field. The formed nanochains were fixed with an additional thin silica layer. The magnetic nanoparticles inside the nanoclusters with a thin silica shell were then dissolved in acid to form nanochains composed of hollow silica shells and the superparamagnetic nanoclusters coated with the thick non-permeable silica. This strategy will make a basis for the further development of new magnetic drug-delivery systems.

In the research led by Institute of Cell Biology, University of Ljubljana, magnetic nanoclusters labelled with two fluorescent dyes, fluorescein and rhodamine were applied for the labelling of urothelial nanotubes. The tunnelling membrane nanotubes are spontaneously formed between urothelial cancer cells to transfer information in the form of genetic material and other cellular building blocks between the cells. An important part of the project was aimed at investigating synthetic approaches for the preparation of small nanoclusters with a size of around 70–80 nm, which is the upper limit for urothelial nanotubes labelling. Additionally, the nanoclusters conjugated with targeting ligands for the recognition of urothelial cancer cells were developed in the frame of the project.

In a recently established collaboration with a research team from the University of Cyprus an encapsulation of the magnetic nanoclusters into polymer electrospun fibres was investigated. The carbon-based nanocomposites obtained with calcination of the fibres were tested as anode materials in Li-ion batteries. In another project the superparamagnetic nanoclusters labelled with fluorescein were applied in the development of new materials for gas sensing.

We continued the research devoted to nanocomposites containing magnetic nanoparticles dispersed in a polymethyl methacrylate polymer matrix. The knowledge developed in this research enabled the preparation of magnetic nanoparticles with liquid-crystal (5CB)-bearing polymer chains at the surfaces. The procedure for their preparation is based on bonding monomer methyl methacrylate onto the surfaces of the magnetic nanoparticles. During the polymerization of the acrylic monomer bearing the 5CB moiety in the presence of the nanoparticles a part of the polymer chains grew from the surface of the nanoparticles. The mixtures of the nanoparticles with the liquid crystals are further studied at the Department of Complex Matter, JSI.

An important part of our research was devoted to BaFe<sub>12</sub>O<sub>19</sub> nanoplatelets. A part of that was dedicated to a determination of their crystal structure. The hexaferrite crystal structure can be represented as a stacking of two

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**An equilibrium structure of barium-hexaferrite nanoplatelets was determined using an atomic-resolution scanning-transmission microscope.**

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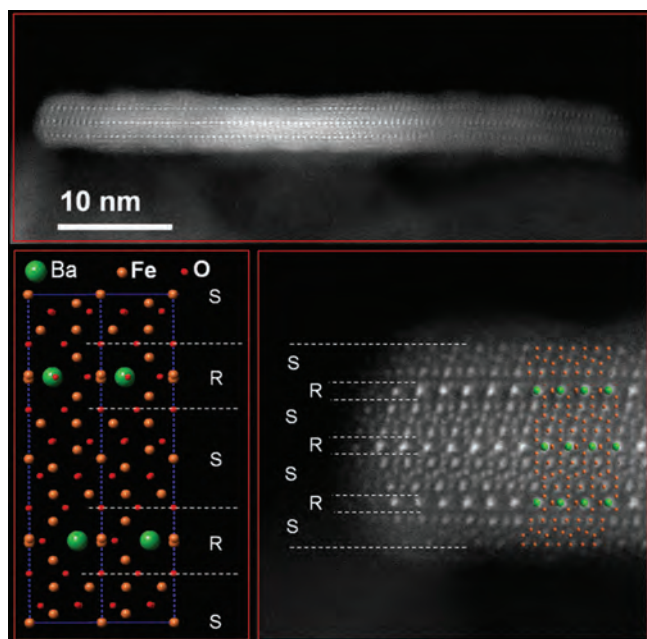


Figure 3: HAADF image of hexaferrite nanoplatelet. Image below shows the structure of hexaferrite along  $[10-10]$ . On a magnified image below, columns containing Ba and Fe atoms are marked.

structural blocks, which alternate along the  $c$ -direction of the hexagonal cell: the hexagonal “R” block ( $(\text{BaFe}^{3+}_6\text{O}^{2-}_{11})^{2-}$ ) and the cubic “S” block ( $(\text{Fe}^{3+}_6\text{O}^{2-}_8)^{2+}$ ). Growth of the hexaferrite crystals is limited in the  $c$ -direction. The hexagonal nanoplatelets, approximately 50 nm wide but only few nm thick, can be synthesized using an appropriate hydrothermal method. Due to the small dimension in the  $c$ -direction of the structure corresponding to their small thickness, the nanoplatelets display a specific structure. The structure of the hexaferrite nanoplatelets was an important topic of our research some years ago. However, even many different methods (high-resolution electron microscopy (HRTEM), x-ray diffractometry (XRD), x-ray adsorption spectroscopy (EXAFS), Mossbauer spectroscopy, etc.) were applied, the structure could not be determined. Only the application of a new, atomic-resolution scanning-transmission electron microscope (ARM) in 2016 enabled a detailed determination of the structure. It appeared that the nanoplatelets display a very uniform structure. A vast majority of the nanoplatelets contain only two hexagonal “R” blocks, or less frequently they contained three “R” blocks. The nanoplatelet structure always terminates with the cubic “S” block (Figure 3). Thus, the thickness of the nanoplatelets is either 3.0 nm for the two “R” blocks, or 4.2 nm for the three “R” blocks. Very seldom were the thicker nanoplatelets, containing four or more “R” blocks, found.

The structure of hexaferrite nanoplatelets is reflected in their unique magnetic properties, defined by their very large, uniaxial magnetic anisotropy with easy axis pointing perpendicular to the platelet. This property enables very effective aligning of the nanoplatelets with an applied magnetic

field, which has been the key to the development of new materials, e.g., ferromagnetic fluids, soft magneto-electrics, or magneto-optic composites, and new applications, especially in medicine.

The disadvantage of the hexaferrite nanoplatelets is in their relatively low saturation magnetization  $M_s$ . As a typical hard-magnetic material the hexaferrite displays a relatively low  $M_s$  of 72 Am<sup>2</sup>/kg in the bulk, whereas in

the form of nanoplatelets the magnetizations are lower. With long-term research we managed to increase the  $M_s$  of the hexaferrite nanoplatelets above 30 Am<sup>2</sup>/kg, however, some applications require even higher magnetizations. The  $M_s$  can be strongly improved by coating nanoplatelets with a shell of iron oxide maghemite ( $\gamma\text{-Fe}_2\text{O}_3$ ), which displays soft-magnetic properties with a relatively high  $M_s$ . If the properties of the two magnetic materials are exchange-coupled, the formed composite nanoplatelet will magnetize homogeneously as a single-phase particle. The hexaferrite core provides the desired large and uniaxial anisotropy, while the surface layer

strongly improves the  $M_s$ . Moreover, the hysteresis shape of the composite nanoplatelets can be precisely adapted to requirements of their application simply with changing the shell thickness.

The maghemite shell is deposited using simple co-precipitation of iron ions from the aqueous solution. The shell is formed after heterogeneous nucleation of the products at the core surfaces. The key factor is control of the supersaturation of the products. The necessary control of the supersaturation was achieved by bonding iron (III) ions into a complex with urea, which enables the controlled release of the ions into the reaction mixture with thermal decomposition of the complex. The research in 2016 was devoted to adaptation of the synthesis procedure to allow close control of the maghemite shell thickness. The thickness can be increased to some extent simply by increasing the concentration of the iron precursors. For thicker shells the coating process had to be repeated several times. The structural properties of the synthesized composite nanoplatelets were analysed using ARM. It appeared that the composite nanoplatelets could be synthesized with exceptional control using our method. They showed incredibly uniform structure, which was to a large extent defined by the uniform structure of the hexaferrite cores. The spinel maghemite layers grow epitactially exclusively at the basal surfaces of the hexaferrite core nanoplatelets (Figure 4). The maghemite surface layers are of uniform thicknesses; the thickness of the layers at the individual core is equal on the both basal surfaces of the core

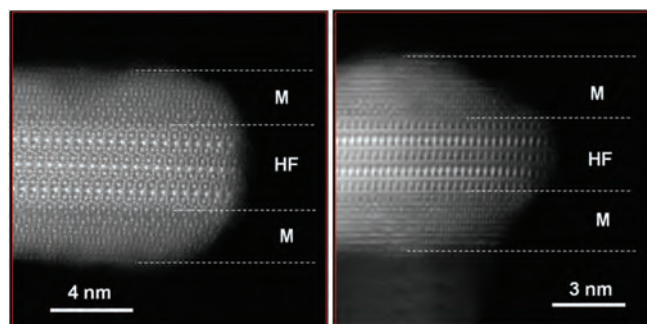


Figure 4: HAADF images of composite nanoplatelets. An individual nanoplatelet is composed of a hexaferrite core (HF) in between of two maghemite layers (M). The hexaferrite core on the left-hand image contains three layers of the  $\text{Ba}^{2+}$  ions (orientation of the core is  $[10-10]_{\text{HF}}$ ), the hexaferrite core on the right-hand image contains two layers of the  $\text{Ba}^{2+}$  ions (orientation of the core is  $[11-20]_{\text{HF}}$ ).

on the level of few atomic layers. The layer thickness also varies minimally when comparing different composite nanoplatelets in the sample.

We also continued the research devoted to applications of hexaferrite nanoplatelets and their incorporation into liquid crystals (in cooperation with the Department of Condensed Matter, JSI). Our studies were focused on modification of the nanoplatelets' surface chemistry. The aim was to increase the concentration of the nanoplatelets in liquid crystals by hydrophobization of their surfaces. This should intensify the magnetic response of the ferromagnetic liquid crystals. In parallel we were involved (with the Department of Condensed Matter, JSI and University of Colorado) in the development of isotropic ferromagnetic liquids, which showed similar behaviour to ferromagnetic liquid crystals. Moreover, the isotropic ferromagnetic liquids showed very high sensitivity to a magnetic field, as they responded to the Earth's magnetic field.

We also participate in the development of novel magnetic-field sensors (in cooperation with Faculty of Electrical Engineering and Computer Science, University of Maribor) through the optimization of nanoplatelet suspensions.

We continued with the research of fluorescent optical materials. Fluorescent nanoparticles with upconversion emission can be applied in various optical elements and are also proposed as alternative bio-markers in imaging diagnostic techniques for medicine. We continued with the studies of the chemical stability of fluoride nanoparticles doped with lanthanides and the development of protective coatings. Namely, the nanoparticles for biomedicine should be chemically and colloidally 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 conducted in cooperation with the Department for Inorganic Synthesis and Technology, JSI, suggested the dissolution mechanism of exemplary  $\text{AlF}_4$  nanoparticles ( $A = \text{Na}$  or  $\text{K}$ ), co-doped with  $\text{Yb}^{3+}$  in  $\text{Tm}^{3+}$  (Figure 5). A partial dissolution of these nanoparticles in water was attributed to the surface dissociation, which proceeds in a few minutes. The subsequent dissolution in water is slow. In contrast to this, fluoride nanoparticles dissolve rapidly in a phosphate buffer. The driving

force of the process is the simultaneous formation of poorly soluble lanthanide phosphates. Considering the presence of phosphates in the cells (nucleic acids, ATP, cell membrane) the fluoride fluorescent nanoparticles as such are not suitable for in-vivo applications. For applications of the fluorescent nanoparticles in medicine we tested different coatings for the protection of the nanoparticles against dissolution. The most efficient protective coating was made with cross-linking poly(maleic anhydride-alt-1-octadecen) (PMAO) with bis(hexamethylene)triamine (BHMT). We showed that the cross-linking between the two polymers in the coating is crucial for the purpose. At the same time, the PMAO-BHMT coatings also enabled excellent colloidal stability of the studied nanoparticles in the water and phosphate buffer, and it showed a beneficial effect on the fluorescence intensity of the nanoparticles.

A study of the effect of the dissolution of fluoride fluorescent upconverting nanoparticles on their optical properties was accomplished in cooperation with Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany, and with the Department for Surface Engineering and Optoelectronics, JSI. We showed that changes of the nanoparticles' surface chemistry induced by their partial dissolution significantly reduced the  $\text{Tm}^{3+}$  fluorescence lifetime. Our results represent a basis for the development of a new, non-destructive analytic method for screening the changes of the surface composition of upconverting fluorescent nanoparticles. Namely, surface chemistry has a significant effect on the optical properties of the upconverting nanoparticles due their large surface-to-volume ratio.

The basic research of semiconducting ceramics was devoted to the origin of a positive temperature coefficient of resistivity (PTCR) in  $\text{BaTiO}_3$  ceramics. We have shown that it is possible to prepare PTC thermistors on the basis of  $\text{BaTiO}_3$  ceramics without donor-doping when a composite containing the mixture of conducting phase and non-conducting phase is formed. Due to dimensional changes in the non-conducting phase at its Curie temperature, disconnections occur in the conductive phase that leads to the PTCR anomaly. In this way, we have succeeded in preparing PTC thermistors with a Curie temperature of 180 °C and a low, room-temperature resistivity of the ferroelectric ceramics based on the system of  $\text{BaTiO}_3$ - $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ . The newly developed material, unlike the materials available in the market, contains no toxic lead.

An extremely steep temperature dependence of the electrical resistivity, i.e., a jump-like form of the dependence, was measured in the composite composed of conducting metal and nonconducting ferroelectric  $\text{BaTiO}_3$ . To the best of our knowledge such a sharp temperature characteristic has not been reported in the literature yet.

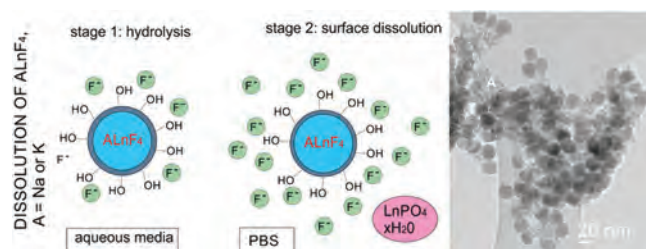


Figure 5: Schematic representation of the dissolution mechanism for fluoride fluorescent nanoparticles (left) and TEM image (right) of nanoparticles in an amorphous phosphate matrix (marked with A), which represents the side product of the dissolution.

## Some outstanding publications in the past year

1. Pušnik, Klementina, Peterlin, Mojca, Kralj Cigić, Irena, Marolt, Gregor, Kogej, Ksenija, Mertelj, Alenka, Gyergyek, Sašo, Makovec, Darko. Adsorption of amino acids, aspartic acid, and lysine onto iron-oxide nanoparticles. *The journal of physical chemistry. C, Nanomaterials and interfaces*, 2016, 120, 14372-14381.
2. Gyergyek, Sašo, Makovec, Darko, Jagodič, Marko, Drogenik, Mihael, Schenk, Kurt, Jordan, Olivier, Kovač, Janez, Dražič, Goran, Hofmann, Heinrich. Hydrothermal growth of iron oxide NPs with a uniform size distribution for magnetically induced hyperthermia : structural, colloidal and magnetic properties. *Journal of alloys and compounds*, 2017, 694, 261-271.
3. Lisjak, Darja, Plohl, Olivija, Vidmar, Janja, Majaron, Boris, Ponikvar-Svet, Maja. Dissolution mechanism of upconverting  $\text{AYF}_4:\text{Yb},\text{Tm}$  (A = Na or K) nanoparticles in aqueous media. *Langmuir*, 2016, 32, 8222-8229.

## Awards and appointments

1. Blaž Belec: 3<sup>rd</sup> award for presentation at the 8. Conference of Jožef Stefan International Postgraduate School, Ljubljana, Jožef Stefan International Postgraduate School.
2. Blaž Belec: Best contribution at the 8. Conference of Jožef Stefan International Postgraduate School, Ljubljana, Jožef Stefan International Postgraduate School.
3. Tanja Goršak: Best presentation at the 8. Conference of Jožef Stefan International Postgraduate School, Ljubljana, Jožef Stefan International Postgraduate School.

## Patent granted

1. Peter Dušak, Marin Berovič, Darko Makovec, Process for regulation of lactic acid fermentation in wine production by magnetic elimination of bacteria, SI24998 (A), Slovenian Intellectual Property Office, 30. 11. 2016

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## INTERNATIONAL PROJECTS

1. COST IC1208; Integrating Devices and Materials: A Challenge for New Instrumentation in ICT  
Prof. Darko Makovec  
Cost Office
2. COST TD1402 - RADIOMAG; Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy  
Prof. Darko Makovec  
Cost Office
3. The European Upconversion Network - From the Design of Photon-Upconverting Nanomaterials to Biomedical Applications  
Prof. Darja Lisjak  
Cost Office

## R&D GRANTS AND CONTRACTS

1. Nanotheranostics based on magneto-responsive materials  
Dr. Slavko Kralj
2. Tunneling nanotubes for innovative urinary bladder cancer treatments  
Dr. Slavko Kralj

## NEW CONTRACTS

1. Development and validation of the TEM method for analysis of an inorganic-core size in final ferric carboxymaltose product  
Prof. Darko Makovec  
Lek d. d.

## RESEARCH PROGRAM

1. Advanced inorganic magnetic and semiconducting materials  
Prof. Darko Makovec

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## VISITOR FROM ABROAD

1. Jan Kotouček, Brno University of Technology, Češka, 1. 8. -9. 9. 2016

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## STAFF

### Researchers

1. Dr. Sašo Gyergyek
2. Prof. Darja Lisjak
3. Prof. Darko Makovec, Head
4. Dr. Igor Zajc

### Postdoctoral associates

5. Dr. Slavko Kralj

### Postgraduates

6. Blaž Belec, B. Sc.
  7. Tanja Goršak, B. Sc.
  8. Dr. Olivija Plohl, left 20.06.16
  9. Dr. Klementina Pušnik, left 19.05.16
- ### Technical and administrative staff
10. Bernarda Anželak, B. Sc.

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1. Slavko Kralj, Tanja Potrč, Petra Kocbek, Silvia Marchesan, Darko Makovec, "Design and fabrication of magnetically responsive nanocarriers for drug delivery", *Curr. med. chem.*, vol. 23, pp. 1-16, 2016.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Blaž Belec, Darko Makovec, "Building thick spinel iron oxide layer onto the hexaferrite core nanoparticles using multiple co-precipitation of iron ions", In: *Zbornik*, 8. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana, 31. maj in 1. junij 2016, Ljubljana, Slovenija, pp. 215-226.
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## PATENT

1. Peter Dušak, Marin Berovič, Darko Makovec, *Process for regulation of lactic acid fermentation in wine production by magnetic elimination of bacteria*, SI24998 (A), Urad RS za intelektualno lastnino, 30. 11. 2016.

## MENTORING

1. Olivija Plohl, *Dissolution of fluoride upconverting nanoparticles in aqueous suspensions and their protection with amphiphilic coatings*: doctoral dissertation, Ljubljana, 2016 (mentor Darja Lisjak).
2. Klementina Pušnik, *Engineering properties of aqueous suspensions of iron-oxide nanoparticles using amino acids*: doctoral dissertation, Ljubljana, 2016 (mentor Darko Makovec).
3. Mojca Peterlin, *Določanje aminokislin adsorbiranih na površini nanodelcev železovega oksida ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>)*: master's thesis, Ljubljana, 2016 (mentor Irena Kralj Cigić; co-mentor Darko Makovec).





# DEPARTMENT FOR ADVANCED MATERIALS

# K-9

***In the Department for Advanced Materials we investigate novel materials through an understanding of the mutual dependence of their structural, microstructural and functional characteristics. Modern technologies that enable the synthesis of materials with atomic and microscale precision are used to prepare pre-designed structural 3D materials, thin films and nanoparticles with the desired crystal structure, chemical composition, microstructure and morphology. Among our important objectives is the development of: i) novel functional oxide materials for various electronic applications, ii) new materials with improved antibacterial and photocatalytic effects and iii) new materials for efficient energy conversion.***

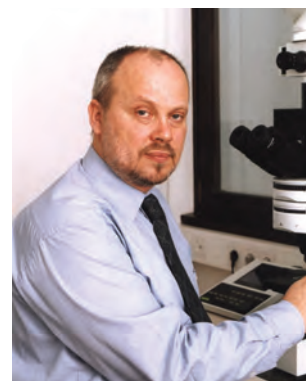
## Functionalized oxides for electronic applications

In our study of the mechanisms for controlling the size of ferroelectric perovskite particles with an anisotropic shape of the plates there were two main directions. In the first part, the main emphasis was on control of the morphology of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  and  $\text{Bi}_{3.8}\text{Nd}_{0.2}\text{Ti}_3\text{O}_{12}$  nanoplates (side length  $\sim 100\text{nm}$ , thickness  $\sim 10\text{nm}$ ) under hydrothermal conditions. The former types of plates were used as the template for a topochemical conversion into perovskite ( $\text{BaTiO}_3$ ,  $\text{SrTiO}_3$ ) nanoparticles with the shape of blocks and plates, while the latter composition was prepared mainly due to a study of their behaviour in a liquid crystal. In the second part, we studied the mechanisms of the topochemical conversion from  $\mu\text{m}$ - and  $\text{nm}$ -sized  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  plates into  $\text{BaTiO}_3$  and  $\text{SrTiO}_3$  in a molten salt or under hydrothermal conditions.

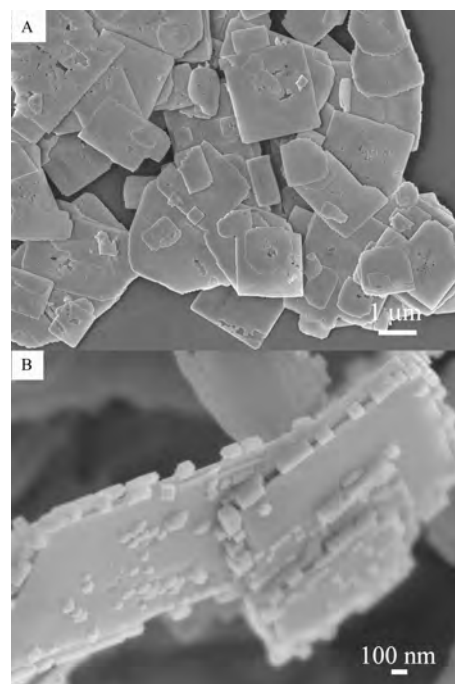
A study of the topochemical conversion of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  nanoplates into  $\text{BaTiO}_3$  in a molten salt was focused on the preservation of the nanodimensions of  $\text{BaTiO}_3$  during heating to high temperature, which is needed for the increase of tetragonality, and consequently the ferroelectricity. For the growth of  $\text{BaTiO}_3$  nano-plates, nano-blocks due to Ostwald ripening were retarded based on the fact that the rate of the dissolution and growth of the particles with flat and smooth faces is slower than those with an irregular shape and high curvature.

The topochemical conversion of layered Aurivillius  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  into  $\text{BaTiO}_3$  or  $\text{SrTiO}_3$  perovskite under hydrothermal conditions has not been reported yet. Previous results imply that it is possible to affect the prevailing growth mechanism and thus tune the reaction towards the target morphology by controlling the synthesis conditions (Figure 1). In order to preserve the anisotropic shape of the  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  plates, the growth of the perovskite on these plates should be layer-by-layer (Frank-van der Merwe). Additionally, it is assumed that control over the reaction conditions for the layer-by-layer growth will also be crucial for the preparation of the composite plates of  $\text{BaTiO}_3/\text{SrTiO}_3$ , which are expected to exhibit enhanced ferroelectric properties due to the lattice strains, which result from the lattice mismatch. Consequently, the ferroelectric polarization of  $\text{BaTiO}_3$  grown on (100) oriented  $\text{SrTiO}_3$  plates is assumed to point perpendicular to the plate surface, which is required in several applications. Ferroelectricity is also expected to be preserved down to smaller dimensions of the  $\text{BaTiO}_3/\text{SrTiO}_3$  nanocomposite plates, which makes them very useful building blocks for the fabrication of nanometric electromechanical devices.

The integration of epitaxial complex oxides with Si represents an invaluable opportunity for the creation of novel devices with logic and sensing capabilities, both implemented in the same chip. Using PLD we grew epitaxial ultra-thin (3–4-nm)  $\text{SrTiO}_3$  (STO) layers on Si(001), showcasing the possibilities of this technique for the growth of templates for the integration of complex oxides with Si. Our procedure involves the growth of a 1/2 monolayer (ML) of Sr buffer layer on the reconstructed Si(001) surface by PLD, the deposition of STO in an inert Ar atmosphere, and latter oxidation and crystallization phases (Figure 2). The optimization of STO deposition, oxidation, and crystallization parameters proves to be essential for the improvement of the layer's quality. It has been found that the minimization of the thermal budget during the crystallization phase increases the interface sharpness, but a minimum temperature is needed for a proper densification of the STO layer. A coverage of 2 ML before every crystallization and oxidation phases was determined as the best balance between the critical thickness, minimization of the thermal budget, and a proper coverage of the buffer layer, which prevents its reactions with the Sr/Si surface. These results improve the general knowledge and understanding of metal oxide/silicon heterojunctions,



Head:  
**Prof. Danilo Suvorov**



**Figure 1:** Topochemical transformation from  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  plate-like particles into  $\text{SrTiO}_3$  under alkaline hydrothermal conditions with the dominance of the growth similar to a) Frank-van der Merwe (layer-by-layer) and b) Volmer-Weber (island formation).

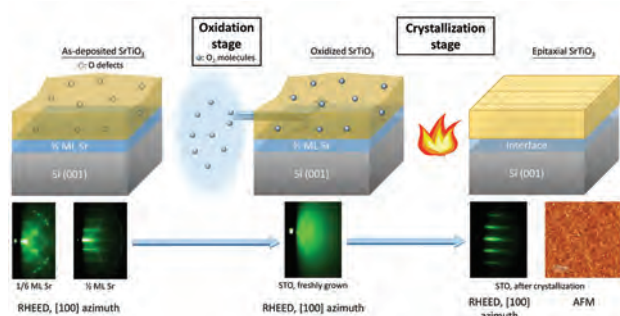


Figure 2: Graphical scheme of the STO growth process. The STO is grown on the 1/2 ML Sr/Si surface, and it consists of STO deposition, oxidation and crystallization phases, which are adjusted to minimize interface reactions and to obtain the most optimal crystalline quality. Below the scheme, RHEED patterns can be seen for the deposition of the Sr buffer layer (left), the freshly grown STO (center) and the crystallized STO (right), along with an AFM image after the final stage of the growth process.

and represent a solid stepping stone for the growth of high-quality, thin STO templates on Si by PLD.

In our work we have studied the structural properties of a strontium buffer layer on silicon grown by the PLD technique. The samples were prepared in a vacuum chamber with a base pressure of  $2 \times 10^{-9}$  by first removing the native  $\text{SiO}_2$  layer by flash annealing at  $1200^\circ\text{C}$ , followed by the deposition of half a monolayer of strontium. *In-situ* characterization by reflection high-energy diffraction showed a typical two-domain  $(2 \times 1) + (1 \times 2)$  reconstruction. In order to ensure an adsorbate-free surface the samples were transferred using an ultra-high vacuum suitcase. The samples were analysed by low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). LEED analysis confirmed that the surface reconstruction was preserved during the transfer. High-resolution STM images revealed a highly ordered surface, which has a quality comparable to a surface prepared using a more established molecular beam epitaxy technique (Figure 3). This study presents the first local structural analysis on of the Sr/Si surface prepared by PLD on the atomic scale.

We used PLD technique to prepare  $\text{Pb}[\text{Mg}_{1/3}\text{Nb}_{2/3}]_2\text{O}_7\text{-PbTiO}_3$  (PMN-PT) thin films on single-crystal  $\text{SrTiO}_3$  substrates as well. PMN-PT exhibits excellent piezoelectrical properties, however, only in the absence of the pyrochlore phase, which can form due to lead-loss during the synthesis. We prepared single-phase PMN-PT films by optimizing the deposition conditions and by using PbO-excess targets. The (001)-peak splitting in the X-ray diffraction spectra revealed a strong influence of the process pressure on the domain structure of the films, which was confirmed by high-resolution transmission electron microscopy. In the next stage we deposited thin-film electrodes ( $\text{SrRuO}_3$  or  $\text{LaNiO}_3$ ) between the STO and the PMN-PT. We found that the electrode layer (especially  $\text{LaNiO}_3$ ) has a pronounced influence on the further growth of PMN-PT by stabilizing the formation of the perovskite phase.

#### Antibacterial and photocatalytic materials

The group for biomaterials has been working on fields including the development of innovative antimicrobial coatings, the development of new antimicrobial biomaterials and innovative techniques for cryopreservation.

We have developed an innovative composite coating system consisting of 1D nanostructured MgO incorporated within the PLGA matrix. We detected the presence of a strong interphase interaction between MgO and PLGA, which resulted in the retention of MgO nanoparticles at the surface of MgO/PLGA coatings. As a consequence, the MgO/PLGA coating was able to prevent *S. epidermidis* colonization without exhibiting any change to the attached red blood cells. We concluded that the stabilization of MgO within PLGA matrix widened the “therapeutic window” of magnesium oxide particles.

We continued our research on nanocomposite materials based on gallium, gold and hydroxyapatite. A nanocomposite of Ga and hydroxyapatite was compared to a nanocomposite of Ag nanoparticles and hydroxyapatite. The new gallium-based nanocomposite was more effective against *Pseudomonas aeruginosa* and less toxic to L929 as well as IMR-90 fibroblasts (Figure 4 and 5). We also investigated the influence of the size and size distribution of the Ga nanoparticle and Ga content on the antibacterial activity and cytotoxicity of the nanocomposite and optimised its synthesis. We could obtain a very narrow size distribution by using oleic acid as a surfactant and thermal decomposition to create Ga nanoparticles. Nanocomposites with such Ga nanoparticles exhibited a stronger antibacterial effect, but also an increased toxicity in comparison with the nanocomposites prepared by ultrasonic emulsification without any surfactant. Based on our discoveries on the incorporation of  $\text{Ga}^{3+}$  ions into hydroxyapatite, we have developed an optimum nanocomposite of functionalised Au nanoparticles and Ga(III)-containing hydroxyapatite, which effectively stops the growth of *P. aeruginosa*, *E. coli* and *S. epidermidis* bacteria and has low toxicity for L929 fibroblasts. Apart from these achievements we have also made very interesting findings about the mechanism and optimisation of the formation of functionalised Ga/Au core-shell nanoparticles and discovered possibilities for their stabilisation. The results of this research, which were published in three research articles, have been selected for an illustration of the Journal of Materials Science: Materials in Medicine.

The research in the field of new biomaterials that combine antimicrobial and magnetic properties was initiated in 2016 in the framework of a bilateral project with Serbia. In this field, we have developed new processes for the synthesis of composites that combine the functionalized nanoparticles of gold (Au-arginine) and ferrite nanoparti-

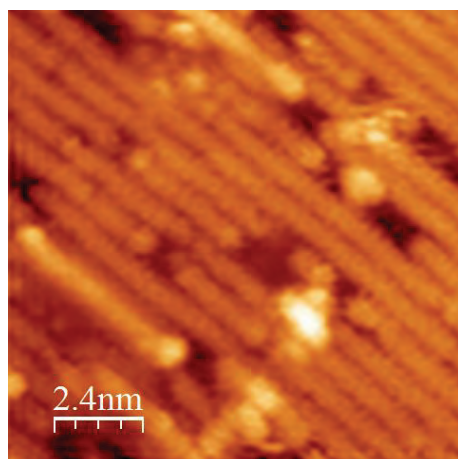


Figure 3: Filled electron state STM image of the Sr/Si(001) surface exhibiting a  $(2 \times 1)$  reconstruction. In the filled electron state image, the tunneling current is related to the Si dangling bonds of the Si dimer chains participating in bonding with Sr atoms sitting in-between the dimer chains ( $T=60\text{ K}$ ,  $U=-3\text{ V}$ ,  $I=200\text{ pA}$ ).

cles ( $MFe_2O_4$ ,  $M = Zn^{2+}, Co^{3+}, Cu^{2+}$ ). We have shown that the new composites possess a strong antimicrobial activity (against *E. coli* and *S. epidermidis*), enabled by functionalized gold, and magnetic properties, which were enabled by ferrite nanoparticles. In spite of the nano-size (20-nm Au particles having 5-nm particles on their surfaces), we showed that the composite particles do not cause damage to blood cells and have shown to be very promising for further research in biomedical applications.

In the field of innovative techniques for cryopreservation we started research on the development of biomimetic inorganic calcium hydroxyapatite (HAp) nanoparticles for the delivery of bioactive payloads in cells. Our research was focused on cell cryopreservation for blood-transfusion applications and the developed HAp nanoparticles were used for the delivery of natural cryoprotectant trehalose in erythrocytes, which lack the endocytosis machinery. The work involved studies of the relationship between nanoparticle properties and their efficiency for trehalose delivery in cells and on the mechanism of interactions between nanoparticles and the cell membrane.

The studies have shown that HAp nanoparticles are efficient agents for the delivery of trehalose in erythrocytes and strongly enhance the cryo-survival of erythrocytes after freeze-thawing. From this area we applied for a Marie Curie research project that was awarded with a “Seal of Excellence” from the European Commission.

### New materials for efficient energy conversion

In the scope on the research on new materials for energy conversion we investigated compounds with a layered crystal structure that comply with the “phonon-glass, electron-crystal” concept and are thus interesting for the development of new thermoelectric materials. In the case of materials based on layered titanium disulphide we developed a process that allows the synthesis of a highly stoichiometric compound, which leads to a wide range of possibilities regarding the formation of intercalated bulk materials with improved electrical and thermal transport properties. Furthermore, we optimized a high-pressure pulsed electric current sintering process that resulted in highly textured, twinned bulk materials based on titanium disulphide with an order of magnitude lower thermal conductivity.

In the case of bulk materials based on layered cobaltates we found that crystal structure changes within individual grains can be triggered by changing the atmosphere in the predicted operating temperature range. The findings contribute to a new understanding of the crystal chemistry of layered compounds as candidate materials for thermoelectric energy conversion.

Within the research field of energy-conversion materials we also studied crystal-structure and domain-texture changes induced by external mechanical stresses and electrical fields. For the studies, we applied *in-situ* X-ray diffraction and *in-situ* transmission electron microscopy to the lead-free piezoceramics. We found that induced changes depend on the initial state of the material. The study contributed to an understanding of the coupling between structural changes, which is crucial for development of new environmentally friendly piezomaterials.

### Materials for heat-insulation applications

Our research focused on the development of insulation materials with improved insulation capacity, temperature stability, and/or improved sustainability. We investigated foaming mechanisms for various glass cullets and identified additives that enable the tuning of the foaming process in the preparation of foam glasses. Selected additives facilitate the preparation of foam glass from cullets of cathode-ray-tube (CRT) panel glass, flat glass, container glass as well as their mixtures under very similar process conditions (Figure 6). A decreased dependence of the foaming process on the composition of the glass is an important scientific and industrial contribution. Foam-glass products with a high content of container glass were open porous, suitable for use in sound insulation. Closed-porous foams are suitable for load-bearing, age-resistant thermal insulation within the whole lifespan of the building. The thermal conductivity of the foams with a higher content of the CRT panel glass (Figure 7) was lower than that of the foams with the container or bottle glass. The lowest achieved thermal insulation values are 39–40 mW/(m·K). We also measured the thermal conductivity of the solid structure in an evacuated open-porous sample, which revealed the approximately 50 % contribution of the solid conductivity to the effective thermal conductivity.

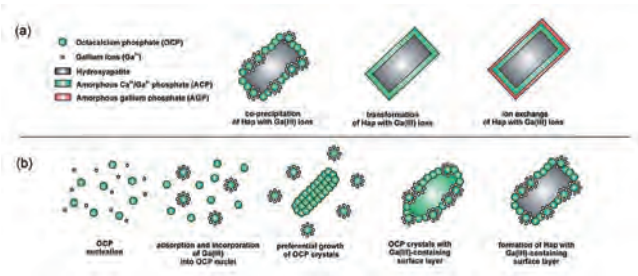


Figure 4: a) Illustration of the structure of HAp(Ga) obtained by co-precipitation, transformation and ion exchange with  $Ga^{3+}$  ions and b) the mechanism of formation of HAp(Ga) co-precipitated nanocrystals.

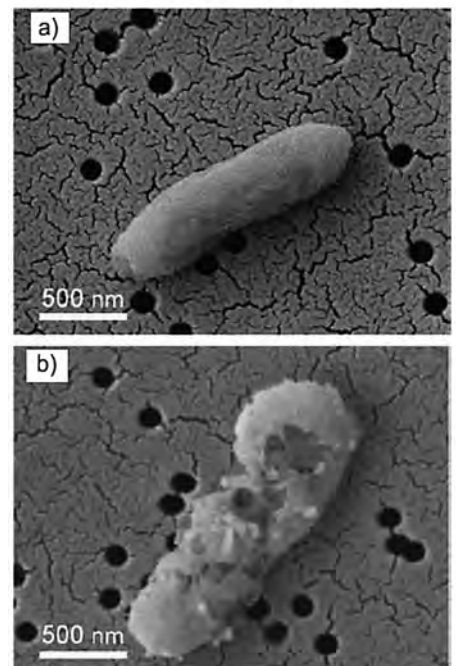


Figure 5: Bacterial morphology: a) SEM image of *P. aeruginosa* MW1 after 24h incubation in growth medium with 0.5 mg/mL hydroxyapatite and b) SEM image of *P. aeruginosa* MW1 after 24h incubation in growth medium with 0.1 mg/mL of Ga@HAP.

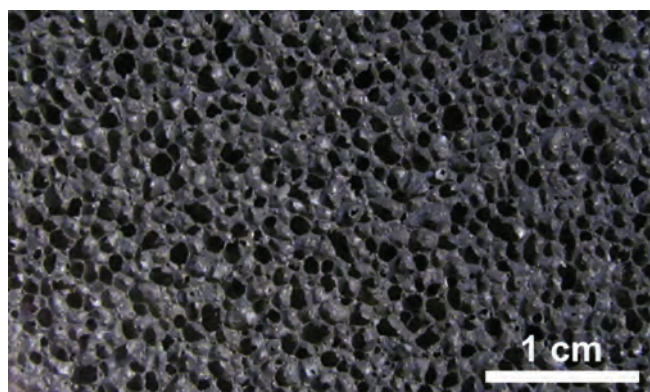


Figure 6: Microstructure of a foam glass with 95 % porosity prepared from waste window glass.

#### ENPIEZO

In the scope of the M-ERA.NET project ENPIEZO we are developing piezo-electric-based energy-harvesting (EH) devices to provide a remote source of electricity from waste vibrations. We are investigating the fabrication-friendly pulsed-laser deposition of high-quality epitaxial  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$  (PMN-PT) thin films on Si, based on the delicate engineering of silicon-oxide interfaces. The study, joining laboratory- and industrial-scale systems, is the first of its kind. On our laboratory system we thoroughly studied the Sr-reconstructed Si surface and optimized the crucial growth parameters of  $\text{SrTiO}_3$  (STO) on Si. Separately, we optimized the growth on PMN-PT thin films on single-crystal STO substrates, whereupon we started integrating the two systems. Within this project we are also studying the preparation of polycrystalline PMN-PT films by aerosol-deposition on stainless-steel substrates. In the past year mathematical modelling of the piezoelectric transducers was also completed. Simultaneously, we investigated various potential applications for these transducers.

#### EPCOS

For our industrial partner EPCOS OHG, Deutschlandsberg, Austria, in the past year we have carried out the project: "Devices for energy storage based on PLZT thin films and Cu electrodes". We grew PLZT thin films using a laboratory and industrial system for pulsed-laser deposition. On Si substrates with a diameter of 150 mm we successfully controlled the chemical homogeneity of all the present elements, as well as the layer thickness along the substrate. Further development of advanced devices for energy storage in electronic applications will be based on the results of this project.

#### SCOPEs

Within the SCOPEs project, which is trilateral cooperation between Serbia, Slovenia and Switzerland, we have developed new methods for forming porous structures which are suitable as carriers of stem cells and are useful in tissue engineering. Such structures include a polymer matrix (made up of a series of new biocompatible and biodegradable polymers, which we developed together with the TMF partner in Serbia) and the inorganic particles are based on doped apatite (which includes ions such as  $\text{Mg}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ga}^{3+}$  and  $\text{Sr}^{2+}$ ). In the first phase of materials testing (which was made in the ETH within a cooperation with a partner in Switzerland), we have shown that the presence of ions has a strong influence on the different stages of the cell life cycle of stem cells and stimulates their differentiation and growth.



Figure 7: Cross-section images of the foam glasses prepared from panel glass powders with different particle sizes. The density of the foam glass prepared from 13- $\mu\text{m}$  powders is 120  $\text{kg}/\text{m}^3$ .

#### CleanTechBlock II

Project CleanTechBlock II - energy-saving facade building component develops and demonstrates a new building block with improved foam glass insulation core and clay brick shells. The goal of the project is to demonstrate the new foam-glass preparation process on a larger scale (size 1:1) and preparation and thermal insulation property testing of a wall segment from the new building blocks.

#### Some outstanding publications in the past year

1. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, "Influence of the glass particle size on the foaming process and physical characteristics of foam glasses", *J. non-cryst. solids*, vol. 447, str. 190-197, 2016, doi: 10.1016/j.jnoncrysol.2016.05.021.
2. Lei Li, Matjaž Spreitzer, Danilo Suvorov, "The microstructure, dielectric abnormalities, polar order and microwave dielectric properties of  $\text{Ag}(\text{Nb}_{1-x}\text{Ta}_x)\text{O}_3$  ( $x = 0-0.8$ ) ceramics", *J. Eur. Ceram. Soc.*, vol. 36, no. 14, str. 3347-3354, 2016, doi: 10.1016/j.jeurceramsoc.2016.05.017.
3. Vojka Žunič, Mario Kurtjak, Danilo Suvorov, "Bifunctional bridging linker-assisted synthesis and characterization of  $\text{TiO}_2/\text{Au}$  nanocomposites", *J. nanopart. res.*, vol. 18, no. 11, str. 336-1-336-11, 2016.
4. Zoran Jovanović, Matjaž Spreitzer, Urška Gabor, Danilo Suvorov, "Control of SrO buffer-layer formation on Si(001) using the pulsed-laser deposition technique", *RSC advances*, vol. 6, issue 85, str. 82150-82156, 2016, doi: 10.1039/c6ra16311d.

- Mario Kurtjak, Marija Vukomanović, Andraž Krajnc, Lovro Kramer, Boris Turk, Danilo Suvorov, "Designing Ga(III)-containing hydroxyapatite with antibacterial activity", RSC advances, vol. 6, iss. 114, str. 112839-112852, 2016, <http://pubs.rsc.org/en/content/articlepdf/2016/ra/c6ra23424k>, doi: 10.1039/C6RA23424K.
- Nemanja Aničić, Marija Vukomanović, Danilo Suvorov, "The nano-texturing of MgO microrods for antibacterial applications", RSC advances, 6(104), str. 102657-102664, 2016, doi: 10.1039/C6RA23058J.

## Awards and Appointments

- Urška Gabor: Award for best oral presentation in young researchers section at the 24th International Conference on Materials and Technology, Portorož, Metals and Technology (IMT), "Different approaches to avoiding lead deficiency in PMN-PT thin films"
- Martin Štefanič: Seal of Excellence, Brussels, Belgium, European Commission, project proposal NanoDryCell: Nanoparticle-assisted desiccation of mesenchymal stem cells for the "off-the-shelf" allogeneic cell therapy

## Organization of conferences, congresses and meetings

- Workshop on M.ERA-NET project "ENPIEZO: Enabling technology for high-quality piezoMEMS", Taipei, Taiwan, 21. - 28. 2. 2016 (co-organizers)
- Workshop on "EUDP Clean TechBlock II" project, Aalborg, Denmark, 29. 2. - 4. 3. 2016 (co-organizers)
- Workshop on M.ERA-NET project "HarvEnPiez: Innovative nano-materials and architectures for integrated piezoelectric energy harvesting application", Ljubljana, 25. - 26. 8. 2016
- Workshop on M.ERA-NET project "ENPIEZO: Enabling technology for high-quality piezoMEMS", Oslo, Norway, 31. 8. - 3. 9. 2016 (co-organizers)
- COST TO-BE (Towards Oxide - Based Electronics) Fall Meeting 2016, Ljubljana, 28. - 30. 9. 2016
24. International Conference on Materials and Technology, Portorož, 28. - 30. 9. 2016 (co-organizers)

## INTERNATIONAL PROJECTS

- Thin-Film-Energy-Storage Device on the basis of PLZT and Cu-Electrodes  
Prof. Danilo Suvorov, doc. dr. Matjaž Spreitzer  
Epcos Ohg
- Investigation of Rare Earth Alloys and Related Compounds  
Prof. Danilo Suvorov, doc. dr. Srečo Škapin  
Urban Mining Company
- Investigation of Rare Earth Alloys and Related Compounds  
Prof. Danilo Suvorov, doc. dr. Srečo Škapin  
Urban Mining Company
- COST MP1308: Towards Oxide Based Electronics (TO-BE)  
Asst. Prof. Matjaž Spreitzer  
Cost Office
- COST 1308 TO BE Workshop, Ljubljana, Slovenia, 28.-30.9.2016  
Asst. Prof. Matjaž Spreitzer  
Cost Office
- Gold/Ferrite Nanocomposites: Antimicrobial and Magnetic Properties for Biomedical Applications  
Marija Vukomanović  
Slovenian Research Agency
- Thermoelectric Materials based on Layered Crystal Structures  
Asst. Prof. Boštjan Jančar  
Slovenian Research Agency

## RESEARCH PROGRAM

- Contemporary Inorganic Materials and Nanotechnologies  
Prof. dr. Danilo Suvorov

## R & D GRANTS AND CONTRACTS

- 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  
Asst. Prof. Matjaž Spreitzer
- Development of heterogeneous catalysts for oxidative dehydrogenation of propane with CO  
Asst. Prof. Matjaž Spreitzer
- SCOPES; Intelligent Scaffolds as a Tool for Advanced Tissue Regeneration  
Marija Vukomanović  
Snf- Swiss National Science Foundation
- Cleantech Block II - Energy Saving Cladding  
Dr. Jakob König  
Eddp (eudp) Energy Technology Development
- Enabling technology for high-quality piezoMEMS  
Asst. Prof. Matjaž Spreitzer  
MIZS

## NEW CONTRACTS

- Development and characterisation of mineral wool fibres  
Prof. Danilo Suvorov, dr. Jakob König  
Knauf Insulation, d. o. o., Škofja Loka
- PBE Silent and PBE Varioface  
Prof. Danilo Suvorov, dr. Jakob König  
Knauf Insulation, d. o. o., Škofja Loka

## VISITORS FROM ABROAD

- Jelena Mitrić, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 21.11. - 25.12.2016
- Dr. Zoran Jovanović, Dr. Sonja Jovanović, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 18.11. - 23.12.2016
- Prof. Xiang Ming Chen, Institute of Materials Physics, School of Materials Science and Engineering, Zhejiang University, Hangzhou, China, 26. - 31. 8. 2016
- Dr. Ioana Vlaicu, Dr. Raluca Negrea, National Institute of Materials Physics, Bucharest, Romania, 25. - 26. 8. 2016
- Dr. Olga Plopa, Intellectro Iasi SRL, Romania, 25. - 26. 8. 2016
- Dr. Eugene Kotomin, University of Latvia, Riga, Latvia, 25. - 26. 8. 2016
- Dr. Sonja Jovanović, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 24. 7. - 21. 8. 2016
- Dr. Jyoti Prosad Guha, Missouri University of Science and Technology, Rolla, USA, 26.6. - 23. 9. 2016
- Dr. Manfred Schweininger, Dr. Kerstin Schmoltnner, TDK EPCOS, Deutschlandsberg, Austria, 24.6.2016.
- Dr. Maja Dekić, Amra Salčinović, University of Sarajevo, Sarajevo, Bosnia and Herzegovina, 19. - 29.6.2016
- Prof. Yuanzheng Yue, Dr. Rasmus R. Petersen, Martin B. Østergaard, Aalborg University & Jacob H. Bendtsen, Peter Matzen, Gråsten Brickwork, Denmark, 15.6.2016
- Dr. Kerstin Schmoltnner, TDK EPCOS, Deutschlandsberg, Austria, 1. - 2.6.2016
- Dr. Bratislav Antić, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 20. - 23. 4. 2016

14. Dr. Sonja Jovanović, Vinča Institute of Nuclear Sciences, Belgrade, Serbia 12. – 25. 4. 2016
15. Dr. Chao-Ting Chen, National Taiwan University, Taipei City, Taiwan, 20. – 27. 3. 2016

**Visiting Researchers**

1. Dr. Jyoti Prosad Guha, Missouri University of Science and Technology, Rolla, USA, 26.6. – 23. 9. 2016
2. Dr. Daniel Diaz Fernandez, Universidad Autónoma de Madrid, Spain, 1. 10. 2015 – 30. 9. 2017

## STAFF

**Researchers**

1. Asst. Prof. Boštjan Jančar
2. Dr. Jakob König
3. Dr. Špela Kunej
4. Dr. Marjeta Maček Kržmanec
5. Dr. Matjaž Spreitzer
6. Prof. Danilo Suvorov, Head
7. Asst. Prof. Srečo Davor Škapin
8. Dr. Marija Vukomanović

**Postdoctoral associates**

9. Dr. Mojca Otoničar, 01.05.16, transferred to Department K5
10. Dr. Martin Štefanič
11. Dr. Vojka Žunič, left 01.04.16

**Postgraduates**

12. Nemanja Aničić, B. Sc.

13. Alja Čontala, B. Sc.
14. Urška Gabor, B. Sc.
15. Mario Kurtjak, B. Sc., left 01.09.16
16. Tjaša Parkelj, B. Sc.
17. Tilen Sever, B. Sc.

**Technical officers**

18. David Fabijan, B. Sc.
19. Dr. Jana Ferčič, left 01.07.16
20. Damjan Vengust, B. Sc.

**Technical and administrative staff**

21. Vesna Butinar, B. Sc.
22. Maja Šimaga, M. Sc., 01.12.16, transferred to Department B3
23. Silvo Zupancič

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### ORIGINAL ARTICLE

1. Nemanja Aničić, Marija Vukomanović, Danilo Suvorov, "The nano-texturing of MgO microrods for antibacterial applications", *RSC advances*, vol. 6, iss. 104, pp. 102657-102664, 2016.
2. Marja Jerič, Johannes de Boor, Boštjan Jančar, Miran Čeh, "An enhanced thermoelectric figure of merit for Sr(Ti<sub>0.8</sub>Nb<sub>0.2</sub>)O<sub>3</sub> based on a Ruddlesden-Popper-polytype-induced microstructure", *J. Eur. Ceram. Soc.*, vol. 36, no. 5, pp. 1177-1182, 2016.
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4. Luka Kelhar, Jana Bezjak, Pascal Boulet, Marjeta Maček, Sašo Šturm, Martin Lamut, Boštjan Markoli, Spomenka Kobe, Jean-Marie Dubois, "Stabilisation of Ce-Cu-Fe amorphous alloys by addition of Al", *Philos. mag.* (2003), vol. 96, iss. 30, pp. 3143-3185, 2016.
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6. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, "Influence of the glass particle size on the foaming process and physical characteristics of foam glasses", *J. non-cryst. solids*, vol. 447, pp. 190-197, 2016.
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8. Mario Kurtjak, Marija Vukomanović, Lovro Kramer, Danilo Suvorov, "Biocompatible nano-gallium/hydroxyapatite nanocomposite with antimicrobial activity", *J. mater. sci., Mater. med.*, vol. 27, iss. 11, art. 170, 2016.
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"Microwave properties of sphere-, flake-, and disc-shaped BaFe<sub>12</sub>O<sub>19</sub> nanoparticle inks for high-frequency applications on printed electronics", *J. magn. magn. mater.*, vol. 419, pp. 218-224, 2016.

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### PUBLISHED CONFERENCE CONTRIBUTION

1. Aysen Kaya, Matejka Podlogar, Damjan Vengust, Damjan Svetin, Süleyman Kahraman, Aleksander Rečnik, Slavko Bernik, "Hydrothermal growth of doped ZnO films on amorphous substrates", In: *Conference proceedings 2016*, 52nd International Conference on Microelectronics, Devices and Materials and the Workshop on Biosensors and Microfluidics, September 28 - 30 2016, Ankarana, Slovenia, pp. 37-42

# 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 in 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.

We have continued with proteomic approaches devoted to the identification of protease specificities and the identification of physiological protease substrates. We have thus developed a novel, in-gel-based method that allows a very rapid determination of protease specificities and was already successfully tested on a few proteases, including trypsin and several cysteine cathepsins. In addition, we have in collaboration with dr. O. Schilling (University of Freiburg) developed an improved gel-based approach for the identification of protease substrates. In this approach peptide libraries are generated by the endoproteolytic digestion of proteomes without chemical modification of the primary amines before exposure to a protease under investigation. After incubation with a test protease, treated and control libraries are differentially isotope-labelled and analysed by liquid chromatography-tandem mass spectrometry. We validated the workflow with trypsin and caspase-3, and additionally provided specificity profiles of a protease encoded by a human endogenous retrovirus and for chlamydial protease-like activity factor, as well as for a disintegrin and metalloproteinases with thrombospondin motifs (ADAMTS) -4, -5, and -15, where we showed a canonical profile, including glutamate in P1 and glycine in P3' positions.

We have previously demonstrated that cysteine cathepsins can facilitate the proteolytic release of the extracellular domains of several transmembrane proteins (ectodomain shedding), which is one of the major mechanism in regulating cellular signalling. In collaboration with dr. Dennis Thiele (Duke University), we identified Ctr1, a high-affinity Cu (+) transporter on the plasma membrane and endosomes that exists as a full-length protein and a truncated form of Ctr1 lacking the methionine- and histidine-rich metal-binding ectodomain with reduced Cu (+) transport activity, as a substrate of cathepsins L and B *in vivo*. We were also invited to write an overview on current proteomic and degradomic approaches and challenges in identifying protease substrates and specificities with a special focus on terminomic strategies, which combine peptide labelling and enrichment.

In addition to proteomic approaches, we also worked on small-molecule substrates and probes. The major enzyme we focused on was legumain (AEP), which is linked to a number of diseases including inflammation, arteriosclerosis, and tumorigenesis. In collaboration with dr. M. Drag (University of Wroclaw), we used a hybrid combinatorial substrate library (HyCoSuL) approach to obtain P1-Asp fluorogenic substrates and biotin-labelled inhibitors that targeted legumain. Since this approach led to probes that were also recognized by caspases, we introduced a Counter Selection Substrate Library (CoSeSuL) approach that biases the peptidic scaffold against caspases, thus delivering highly selective legumain probes, which were successfully validated in cells. This approach offers several advantages in the design of selective probes for proteases where the selectivity is difficult to achieve using conventional profiling approaches.



Head:  
**Prof. Boris Turk**



Figure 1: Quantum FX micro CT apparatus (Perkin Elmer) enables CT imaging of small rodents in preclinical investigations



We also continued to work on targeted drug-delivery systems and developed several cathepsin B-specific DARPins that have the potential for non-invasive diagnostic imaging and theranostic applications. We also collaborated with dr. G. Blum (Hebrew University, Jerusalem) on the development of reactive drug carriers with a focus on self-assembled tetra-peptides that include the diphenylalanine motif, thereby serving as substrates of the cathepsins. The degradation of such tetrapeptide substrate nanofibers by cathepsin B led to the release of the majority of the incorporated anti-cancerous drug Doxorubicin from the nanofibers. Moreover, we also demonstrated that tumour lysates fully degraded such nanofibers, suggesting that tetrapeptide substrates that form nanostructures could serve as a promising platform for targeted drug delivery to pathologies in which the protease activity is highly elevated.

Another protease that we focused on was cathepsin K, which is a major target in the osteoporosis treatment. We characterized its allosteric fine-tuning via a recently identified allosteric site. We showed that one of the compounds investigated bound to this site and acted as a specific partial inhibitor of the collagenolytic activity of cathepsin K. The allosteric site was further characterized by site-directed mutagenesis and shown that it is involved in specific regulation of the collagenolytic activity of cathepsin K.

Part of the work was also focused on cathepsin L. Insight into the specificity of this protease is important for elucidating its physiological roles and drug discovery. To study interactions with synthetic ligands, we prepared a presumably inactive mutant and crystallized it. Unexpectedly, the crystal structure determined at 1.4 Å revealed that the cathepsin L molecule is cleaved, with the cleaved region trapped in the active site cleft of the neighbouring molecule. Hence, the catalytic mutant demonstrated low levels of catalytic activity, which is unusual for the cathepsins.

Part of the work was also devoted to inhibitors. One of these is the p41 splice variant of the MHC class II-associated chaperone, called the invariant chain p41 Ii, which contains an amino acid sequence, the p41 fragment, which is a thyropin-type inhibitor of proteolytic enzymes. We found that the exogenous p41 fragment can enter the endocytic pathway of targeted human immature DC, where it could inhibit the enzymatic activity of cysteine proteases. In addition, the p41 fragment was shown to reduce the secretion of interleukin-12 during the subsequent maturation of the treated DC. These findings thus support the immunomodulatory potential of the inhibitor. In addition, we have shown that the deletion of the cystatin C gene has an impact on the development of mammary gland carcinomas *in vivo* in a mouse model.

A special honour was given to V. Turk, who was invited together with J. Neefjes and E. Unanue, to write an overview about the MHC class II (MHC-II) molecules, which are critical in the control of many immune responses, including in most autoimmune diseases and other pathologies, and the associated proteolysis. This process ultimately determines the MHC-II-presented peptidome, including cryptic peptides, modified peptides, and other peptides that are relevant in autoimmune responses. The authors illustrated that MHC-II is variable not only in amino acids (polymorphic) but also in its biology, with important consequences for both health and disease. The work was published in *Annu Rev Immunol*, the premier journal in the field.

An important overview about the cathepsins and their regulation in neuronal system was also written by V. Stoka and colleagues, and was published in a special issue of one of the leading journals in neurology, *Aging Res Rev*, which was devoted to the lysosomal system.

Part of the activities was also devoted to other enzymes or associated with our expertise in the field of mass spectrometry and structural biology. In collaboration with colleagues from the National Institute of Chemistry (dr. M. Novič) we used *in-silico* prediction tools to study the substrate or ligand (inhibitor) binding regions of autolysin E, a bacteriolytic enzyme that plays an important role in the division and growth of bacterial cells and therefore represents a promising potential drug target. Combining several approaches, specific amino acid residues were predicted as ligand binding residues. Therefore, the molecules that would bind with inhibitory potency to these residues could represent potential new antibacterial agents. In another collaboration with colleagues from AciesBio (dr. G. Kosec) and the National Institute of Biology (dr. K. Gruden), we have undertaken an integrated study of the genomic, transcriptomic, and proteomic differences between the wild type strain and the industrial high-producing strain of *S. erythraea* to reveal the mechanisms related to increased yield of production of erythromycin. A total of 165 observed mutations led to differences in gene expression profiles and protein abundance between the two strains, which were most prominent in the initial stages of erythromycin production. Enzymes involved in erythromycin biosynthesis, metabolism of branched chain amino acids and proteolysis were most strongly upregulated in the HP strain. Interestingly, genes related to the TCA cycle and DNA-repair were downregulated. Additionally, comprehensive data analysis uncovered significant correlations in the expression profiles of the erythromycin-biosynthetic genes, other biosynthetic gene clusters and previously unidentified putative regulatory genes. Based on this information, we demonstrated that the overexpression of several genes involved in an amino acid metabolism can contribute to an increased yield of erythromycin, confirming the validity of our systems biology approach. Our comprehensive omics approach, carried out in industrially relevant conditions, thus enabled the identification of key pathways affecting the erythromycin yield, suggesting strategies for a rapid increase in the production of secondary metabolites in an industrial environment.

It is worth mentioning that our department has, partially through the help of Center of Excellence Center 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, a proteomics platform and a whole-body imaging platform, based on an IVIS Spectrum imaging system and a Quantum FX micro CT, which was installed in 2016. 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 involved in the Slovenian Center of Excellence CIPKEBIP that we coordinate. 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, Hungary and Japan, which resulted in joint publications.

In addition, B. Turk co-organized together with dr. F.X. Aviles (University Autonomous Barcelona) a B-debate series symposium "Imaging for Life: From Molecules to Diagnostics and Therapy", and several members of the department were invited to give lectures at international symposia and foreign universities.

## Some outstanding publications in the past year

1. Stoka V, Turk V, Turk B. (2016) Lysosomal cathepsins and their regulation in aging and neurodegeneration. *Ageing Res Rev.* 32, 22-37. doi: 10.1016/j.arr.2016.04.010.
2. Unanue ER, Turk V, Neefjes J. (2016) Variations in MHC Class II Antigen Processing and Presentation in Health and Disease. *Annu Rev Immunol.* 34, 265-297. doi: 10.1146/annurev-immunol-041015-055420.
3. Sosnowski P, Turk D. (2016) Caught in the act: the crystal structure of cleaved cathepsin L bound to the active site of Cathepsin L. *FEBS Lett.* 590, 1253-1261. doi: 10.1002/1873-3468.12140.
4. Novinec M, Rebernik M, Lenarčič B. (2016) An allosteric site enables fine-tuning of cathepsin K by diverse effectors. *FEBS Lett.* 590, 4507-4518. doi: 10.1002/1873-3468.12495.

## Organisation of conferences, congresses and meetings

1. 32nd Winter School on Proteases and their Inhibitors, Tiers, Italy, 24 - 28 Februar 2016, coorganisers
2. IUBMB Symposium on Proteinases, Inhibitors and Biological Control, Portorož, Slovenija, 17 - 21 September 2016

## 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)  
Boris Turk  
Cost Office
4. COST OC-2015; TRANSAUTOPHAGY: European Network of Multidisciplinary Research and Translation of Autophagy Knowledge  
Prof. Eva Žerovnik  
Cost Office
5. COST CA 15203; Mitochondrial Mapping: Evolution-Age-Gender-Lifestyle-Environment  
Asst. Prof. Nataša Kopitar - Jerala  
Cost Office
6. COST CA15124; NEUBIAS - A New Network of European Bioimage Analysts to Advance Life Science Imaging  
Asst. Prof. Tina Zavašnik Bergant  
Cost Office
7. COST CA15214; An Integrative Action for Multidisciplinary Studies on Cellular Structural Networks  
Asst. Prof. Nataša Kopitar - Jerala  
Cost Office
8. MD Simulations of the Initial Steps in Oligomerization of an Amyloidogenic Protein Human Stefin B; Complex of Stefin B Oligomers with A-beta  
Prof. Eva Žerovnik  
Slovenian Research Agency
9. Building Interface between Crystallographic Software MAIN and Integrative Modeling Platform IMP  
Prof. Dušan Turk  
Slovenian Research Agency
10. Effect of Anti-oxidants on Protein Aggregation; In Vitro Study of Amyloid Fibrillation on

the Model of Stefin B and Beta2-microglobulin  
Prof. Eva Žerovnik  
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. Nitroxoline and its derivatives as new antitumour drugs  
Asst. Prof. Olga Vasiljeva
2. Role of cysteine cathepsins in inflammation-associated diseases  
Prof. Boris Turk
3. Structural insight into iodine metabolism  
Dr. Ajda Taler-verčič
4. „Insights into the protein interactions involved in the Potato virus Y potatorelation“  
Prof. Dušan Turk
5. Role of cysteine proteases in the process of cancerogenesis  
Prof. Marko Fonović
6. Proteases in inflammation and cell death  
Prof. Boris Turk
7. The role of micro RNA-21 and cathepsins in delayed preconditioning to acute kidney injury  
Prof. Boris Turk
8. XVth International Symposium on Proteinases, Inhibitors and Biological Control, Portorož, Slovenia, 17.9.-21.9.2016  
Boris Turk
9. In Vivo Studies of Antitumor Activity and Toxicity of Low-Dimensional Al-Hydroxide based Nanostructures  
Boris Turk  
National Research Tomsk

## NEW CONTRACT

1. Mass spectrometry analysis  
Prof. Boris Turk  
Krka, Tovarna Zdravil, d. d.

## VISITORS FROM ABROAD

1. Andrey Kadin, Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Science, Moscow, Russia, 1 January - 31 July 2016 (IJS fellowship holder)
2. Prof. dr. Igor Weber, Ruder Bošković Institute, Zagreb, Croatia, 28 February - 12 March 2016
3. Prof. dr. Peter Hamar, Semmelweis University, Department of Pathophysiology, Budapest, Hungary, 16 - 18 April 2016
4. Dr. Vitalie Rotari, Chisinau, Moldova, 1 - 4 Jun 2016
5. Samra Hasanbašić, Univerzitet Tuzla, Bosnia and Herzegovina, 4 July - 3 August 2016
6. Alma Jahić, Univerzitet Tuzla, Bosnia and Herzegovina, 5 September - 4 October 2016
7. Prof. dr. Selma Berbić, Univerzitet Tuzla, Bosnia and Herzegovina, 10 - 14 October 2016
8. Prof. dr. Carlos Lopez Otin, Departamento de Bioquímica y Biología molecular, IUOPA, Universidad de Oviedo, Spain, 16 September 2016
9. Prof. dr. Hiroshi Nakanishi in prof.dr. Wu Zhou, Department of Pharmacology and Aging Science, Faculty of Dental Science, Kyushu University, Fukuoka, Japan, 21 - 22 September 2016
10. Prof. dr. Ozaki Yasuhiko, Department of Obstetrics and Gynecology, Nagoya City University, Graduate School of Medical Sciences, Nagoya, Japan, 22 September 2016
11. prof. dr. Goto Shinobu, Nagoya City Hospital, Department of Obstetrics and Gynecology, Nagoya, Japan, 22 September . 2016
12. prof. dr. Dieter Bromme in Panwar Preety, The University of British Columbia, Vancouver, Canada, 22 September 2016
13. Prof. dr. Henry Chapman, Universitat Hamburg, Germany, 25 - 27 October 2016
14. Prof. dr. Kazuo Umezawa, Department of Molecular Target Medicine Screening, School of Medicine, Aichi Medical University, Nagakute, Japan, 16 - 18 November 2016

## STAFF

### Researchers

1. Dr. Iztok Dolenc
2. Prof. Marko Fonović
3. Asst. Prof. Nataša Kopitar - Jerala
4. Prof. Brigita Lenarčič\*
5. Asst. Prof. *Urška Repnik*, left 14.10.16
6. Prof. Veronika Stoka
7. Andrej Šali, B. Sc.
8. Prof. Boris Turk, Head
9. Prof. Dušan Turk
10. Asst. Prof. Livija Tušar
11. Asst. Prof. Olga Vasiljeva
12. Asst. Prof. Tina Zavašnik Bergant
13. Prof. Eva Zerovnik

### Postdoctoral associates

14. Dr. Miha Butinar
15. Dr. Maruša Hafner Česen
16. Dr. Nataša Lindič
17. Dr. *Katarina Pegan*, left 01.05.16
18. Dr. Jure Pražnikar\*
19. Dr. Vida Puizdar
20. Dr. *Jelena Rajković*, on leave 01.06.16
21. Dr. Barbara Sobotič
22. Dr. Ajda Taler-Verčič
23. Dr. Aleksandra Usenik
24. Dr. Matej Vizovišek

### Postgraduates

25. Monika Biasizzo, B. Sc.

26. *Katja Bidovec*, B. Sc., left 09.06.16
  27. Janja Božič, B. Sc.
  28. Andreja Bratovš, B. Sc.
  29. Marija Grozdanič, B. Sc.
  30. Katarina Hočevar, B. Sc.
  31. Aleksander Krajnc, B. Sc.
  32. Lovro Kramer, B. Sc.
  33. Jure Loboda, B. Sc.
  34. *Sabina Ott*, B. Sc., 01.05.16, transferred to Department B2
  35. Sara Pintar, B. Sc.
  36. Mojca Trstenjak Prebanda, B. Sc.
  37. Dr. Robert Vidmar
  38. Janja Završnik, B. Sc.
- Technical officers**
39. Marjeta Arnolj, B. Sc.
  40. Andreja Sekirnik, B. Sc.
  41. Ivica Stefe, B. Sc.
- Technical and administrative staff**
42. Maja Orehek, B. Sc.
  43. Dejan Pelko
  44. Polonca Pirš Kovačič
  45. *Gregor Pretnar*, left 01.05.16
  46. Barbara Vrtačnik

Note:

\* part-time JSI member

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Martin L. Binossek *et al.* (13 authors), "Identification of protease specificity by combining proteome-derived peptide libraries and quantitative proteomics", *Molecular & cellular proteomics*, vol. 15, pp. 2515-2524, 2016.
2. Lachlan W. Casey *et al.* (13 authors), "The CC domain structure from the wheat stem rust resistance protein Sr33 challenges paradigms for dimerization in plant NLR proteins", *Proc. Natl. Acad. Sci. U. S. A.*, vol. 113, no. 45, pp. 12856-12861, 2016.
3. Sara Drmota Prebil, Urška Slapšak, Miha Pavšič, Gregor Ilc, Vid Puž, Euripedes de Almeida Ribeiro, Dorothea Anrather, Markus Hartl, Lars Backman, Janez Plavec, Brigita Lenarčič, Kristina Djinović Carugo, "Structure and calcium-binding studies of calmodulin-like domain of human non-muscle  $\alpha$ -actinin-1", *Scientific reports*, vol. 6, pp. 1-13, 2016.
4. Javier Fernandez-Martinez *et al.* (17 authors), "Structure and function of the nuclear pore complex cytoplasmic mRNA export platform", *Cell (Cambridge)*, issue 5, vol. 167, pp. 1215-1228, 2016.
5. Katarina Karničar, Igor Drobnak, Marko Petek, Vasilka Magdevska, Jaka Horvat, Robert Vidmar, Špela Baebler, Ana Rotter, Polona Jamnik, Štefan Fujs, Boris Turk, Marko Fonović, Kristina Gruden, Gregor Kosec, Hrvoje Petković, "Integrated omics approaches provide strategies for rapid erythromycin yield increase in *Saccharopolyspora erythraea*", *Microb Cell Fact*, vol. 15, no. 93, pp. 1/17-17/17, 2016.
6. Mario Kurtjak, Marija Vukomanović, Andraž Krajnc, Lovro Kramer, Boris Turk, Danilo Suvorov, "Designing Ga(III)-containing hydroxyapatite with antibacterial activity", *RSC advances*, vol. 6, iss. 114, pp. 112839-112852, 2016.
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  9. Marko Novinec, Mateja Rebernik, Brigita Lenarčič, "An allosteric site enables fine-tuning of cathepsin K by diverse effectors", *FEBS lett.*, vol. 590, iss. 24, pp. 4507-4518, 2016.
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  12. Marcin Poreba *et al.* (11 authors), "Counter selection substrate library strategy for developing specific protease substrates and probes", *Chemistry & Biology*, vol. 23, issue 8, pp. 1023-1035, 2016.
  13. Urška Potočar, Samo Hudoklin, Mateja Erdani-Kreft, Janja Završnik, Krešimir Božikov, Mirjam Fröhlich, "Adipose-derived stem cells respond to increased osmolarities", *PLoS one*, vol. 11, iss. 10, pp. 1-18, Oct. 2016.
  14. Urška Repnik, Maruša Hafner Česen, Boris Turk, "The use of lysosomotropic dyes to exclude lysosomal membrane permeabilization", *Cold Spring Harb. protoc.*, 2016, iss. 5, prot087106.
  15. Urška Repnik, Maruša Hafner Česen, Boris Turk, "Measuring cysteine cathepsin activity to detect lysosomal membrane permeabilization", *Cold Spring Harb. protoc.*, 2016, iss. 5, prot087114.
  16. Urška Repnik, Maruša Hafner Česen, Boris Turk, "Strategies for assaying lysosomal membrane permeabilization", *Cold Spring Harb. protoc.*, 2016, iss. 6, top077479.
  17. Urška Repnik, Maruša Hafner Česen, Boris Turk, "Studying lysosomal membrane permeabilization by analyzing the release of preloaded BSA-gold particles into the cytosol", *Cold Spring Harb. protoc.*, 2016, iss. 6, prot087122.
  18. Piotr Sosnowski, Dušan Turk, "Caught in the act: the crystal structure of cleaved cathepsin L bound to the active site of Cathepsin L", *FEBS lett.*, vol. 590, no. 8, pp. 1253-1261, 2016.
  19. Tanja Špec, Sebastijan Peljhan, Jana Vidič, Nika Lendero Krajnc, Marko Fonovič, Črtomir Tavzes, Polonca Ropret, "CIM [registered sign] monolith chromatography-enhanced ELISA Detection of proteins in Artists' paints: Ovalbumin as a case study", *Mirochem. j.*, vol.127, pp. 102-112, 2016.
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  21. Livija Tušar, Irena Leonida Kropf, Avreljia Cencič, "Impact of salt reduction on the number of microorganisms and a sensory analysis for Kranjska sausages during their shelf-life", *Agricultura*, vol. 13, no. 1-2, str. 33-47, 2016.
  22. Kenneth R. Wong, Elizabeth Memendez, Charles S. Craik, Michael C. Kavanaugh, Olga Vasiljeva, "In vivo imaging of protease activity by Probody therapeutic activation", *Biochimie (Paris)*, vol. 122, pp. 62-67, 2016.
  23. Tina Zavašnik-Bergant, Martina Bergant Marušič, "Exogenous Thyropin from p41 Invariant chain diminishes cysteine protease activity and affects IL-12 secretion during maturation of human dendritic cells", *PLoS one*, vol. 11, no. 3, pp. 0150815-1-0150815-26, 2016.
  24. Janez Žibert, Jure Cedilnik, Jure Pražnikar, "Particulate matter (PM10) patterns in Europe: an exploratory data analysis using non-negative matrix factorization", *Atmos. environ. (1994)*, vol. 132, pp. 217-228, 2016.

## REVIEW ARTICLE

1. Daniel J. Klionsky *et al.* (1998 authors), "Guidelines for the use and interpretation of assays for monitoring autophagy", *Autophagy*, vol. 12, no. 1, pp. 1-240, 2016.
2. Veronika Stoka, Vito Turk, Boris Turk, "Lysosomal cathepsins and their regulation in aging and neurodegeneration", *Ageing research reviews*, vol. 32, pp. 22-37, 2016.
3. Matej Vizovišek, Robert Vidmar, Marko Fonovič, Boris Turk, "Current trends and challenges in proteomic identification of protease substrates", *Biochimie (Paris)*, vol. 122, pp. 77-87, 2016.
4. Eva Žerovnik, Nataša Kopitar-Jerala, R. Layfield, "Recent developments in treating Alzheimer's disease", *Journal of Alzheimer's disease & Parkinsonism*, vol. 6, no. 2, art. 1000220, 2016.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Maša Bošnjak, Urška Kamenšek, Aleš Sedlar, Maja Čemažar, Janja Završnik, Boris Turk, Céline Bouquet, Gregor Serša, "Antimetastatic potential in mice after gene therapy with plasmid AMEP", In: *1st World Congress on Electroporation and Pulsed Electric Fields in Biology, Medicine and Food & Environmental Technologies (WC 2015): Portorož, Slovenia, September 6-10, 2015*, (IFMBE proceedings, vol. 53), pp. 219-222.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Maruša Hafner Česen, Veronika Stoka, Boris Turk, "Role of lysosomes in intracellular degradation", In: *Encyclopedia of cell biology*, (Molecular cell biology, volume 1), San Diego, Elsevier, 2016, pp. 612-620.

## MENTORING

1. Nina Frančič, *Sol-gel based layer containing enzyme His<sub>6</sub>-OPH for organophosphate detection*: doctoral dissertation, Ljubljana, 2016 (mentor Aleksandra Lobnik; co-mentor Brigita Lenarčič).
2. Piotr Sosnowski, *Structural insight in the substrate specificity of cathepsins*: doctoral dissertation, Ljubljana, 2016 (mentor Dušan Turk).
3. Robert Vidmar, *Proteomic characterization of legumain and its physiological substrates*: doctoral dissertation, Ljubljana, 2016 (mentor Marko Fonovič).
4. Monika Biasizzo, *Vpliv cistatina C na aktivacijo inflamasona v mišjih makrofagih, pridobljenih iz kostnega mozga*: master's thesis, Ljubljana, 2016 (mentor Boris Turk).
5. Klara Brusar, *Influence of culinary processing on the nitrate levels in potatoes*: master's thesis, Maribor, 2016 (mentor Tomaž Langerholc; co-mentor Livija Tušar).
6. Griša Prinčič, *Načrtovanje in sinteza za EpCAM specifičnih malih molekul*: master's thesis, Ljubljana, 2016 (mentor Brigita Lenarčič; co-mentor Jurij Svete).
7. Nina Strah, *The effect of butylated hydroxyanisole on signaling pathways triggered by TNF-alpha in a human colorectal adenocarcinoma cell line*: master's thesis, Ljubljana, 2016 (mentor Bojan Doljak; co-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.*

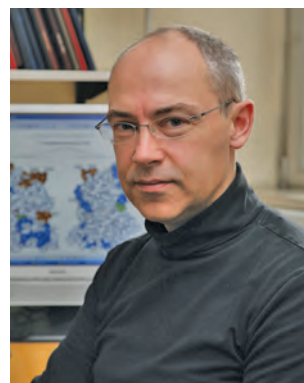
### Toxinology

One of our most important research topics in the field of toxinology is the study of molecular mechanisms for the toxic action of secreted phospholipases A<sub>2</sub> (sPLA<sub>2</sub>) from animal venoms. In particular, we are interested in their presynaptic neurotoxicity. The knowledge that we gather by studying toxic sPLA<sub>2</sub>s represents valuable assistance in understanding the pathophysiological roles of orthologous mammalian sPLA<sub>2</sub>s, for example, their role in the development of neurodegenerative diseases such as Alzheimer's disease.

Ammodytoxin A (AtxA) is a neurotoxic sPLA<sub>2</sub> from the venom of the nose-horned viper (*Vipera ammodytes ammodytes*). In 2016 we continued with the study of the role of the phospholipase activity of this molecule in neurotoxicity. We produced a large amount of a recombinant, enzymatically inactive form of AtxA, AtxA(D49S), and characterized it.

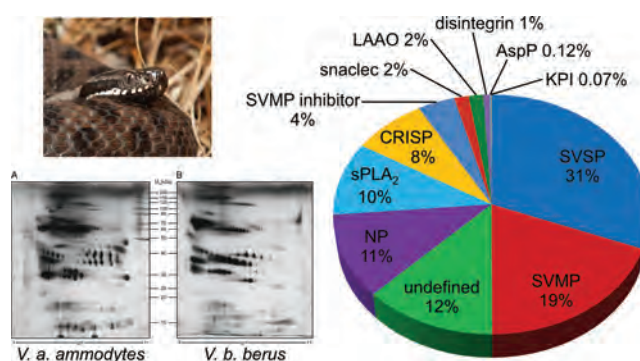
We studied the process of AtxA neurotoxicity using the PC12 model cell line. Mitochondria are the organelles that are the most severely affected by AtxA in nerve cells. We discovered that AtxA binds specifically to cytochrome c oxidase (CCOX) in mitochondria, more precisely, to its catalytic subunit II. We succeeded in demonstrating the interaction between these two proteins also *in vivo* in these cells. Moreover, we showed that AtxA, also as its enzymatically inactive mutant AtxA(D49S), inhibited the oxidation of cytochrome c in mitochondria isolated from PC12 cells and thus pointed to the physiological effect of AtxA on CCOX. We also checked the influence of both sPLA<sub>2</sub> variants on the mitochondrial membrane potential. While AtxA induced its collapse, AtxA(D49S) did not have any effect. The influence on the mitochondrial membrane potential is therefore, contrary to the influence on CCOX, dependent on phospholipase activity. The endogenous sPLA<sub>2</sub>, of the same structural type (group IIA) as AtxA, has been found in mitochondria. Its physiological role in this organelle is still unknown. Our results suggest that this enzyme, through its interaction with CCOX, may be involved in the regulation of cellular respiration. Consequently, deregulation of its function may result in different neurodegenerative diseases, characterized by the malfunction of mitochondria.

In 2016 we continued with the venom proteomics or venomics, the systematic analysis of the components of the nose-horned viper (*Vipera ammodytes ammodytes*) and the common adder (*Vipera berus berus*) venoms. The first comprehensive proteomic results of the common adder venom, very important for the preparation of optimal therapeutic strategy upon envenomation (Figure 1), we succeeded to publish in the respected *Journal of Proteomics* (Z. Latinović et al., *J. Proteomics*, 146 (2016), 34–47). In the past year we also worked intensively on the preparation of a report on the most, to date, inclusive analysis of the nose-horned viper venom that is scheduled for publication in 2017. In the scope of a systematic analysis of the *Vipera a. ammodytes* venom also goes the identification of the cardiotoxic component of this venom. In collaboration with colleagues from the Clinical Department of Infectious Diseases, University Hospital Centre Split, Croatia, and the Department of Pharmacology, Mostar University School of Medicine, Bosnia and Herzegovina, we performed and published an analysis of the effects of all venom fractions on the isolated rat heart (S. Karabuva et al., *Toxicon*, 121 (2016), 98–104). The most prominent effect on the heart was obtained with the venom fraction containing sPLA<sub>2</sub>. We will prepare all the components of this venom fraction in a pure form to define those that are cardiotoxic and describe details of their interference with heart rate.



Head:  
**Prof. Igor Krizaj**

**Animal venoms are a rich source of new substances and molecular tools to improve human and animal health.**



**Figure 1: Comparative venomomics of the two medically most important European vipers.** We have analysed the venom proteome of *Vipera berus berus* (*V.b.berus*) (right-hand part of the figure), the most widely distributed venomous snake in Europe (upper-left part of the figure), and compared it with the venom proteome of the most venomous viper in Europe, *Vipera ammodytes ammodytes* (*V.a.ammodytes*) also using two-dimensional gel electrophoresis (lower-left part of the figure). Obtained results provided an explanation for the effectiveness of treatment of *V.b.berus* envenomation by *V.a.ammodytes* antiserum and explained why full protection of *V.a.ammodytes* venom poisoning by *V.b.berus* antiserum should not always be expected.

With intensity we studied the nose-horned viper venom proteins that affect the blood coagulation process—haemostasis, in particular two such proteins, a homologue of serine protease with anticoagulant activity (VaaSPH-1) and a serine protease with procoagulant, FVIIa-like activity (SP-10). In the past year both molecules were extensively characterized. We determined the complete cDNA sequence of VaaSPH-1. Consequently, we also know its complete amino acid sequence. We started to develop a procedure to produce this protein in mammalian cells. In the case of SP-10, we still do not know its complete cDNA and protein structures. In collaboration with the group of Dr.

Manjunatha R. Kini, the renowned expert for haemostasis from the National University of Singapore, in 2016 we made a major step forward in analysing the molecular mechanisms of VaaSPH-1 and SP-10. Both molecules have special properties and are therefore very interesting for further developments in the direction of medical usage: VaaSPH-1, as a strong inhibitor of blood coagulation without an enzymatic activity, and SP-10, as the first snake venom serine protease that specifically activates FX.

We wrote the first article about disintegrins from the nose-horned viper, which is now in the revision process. Disintegrins are polypeptides that bind to integrin molecules and impair in this way their function. The nose-horned viper disintegrins efficiently prevent migration and thus the spreading of cancer cells. They thus express an anti-metastatic potential, which gives a good prospective for their development in the direction of a new anti-cancer drug.

Following a break, in 2016 we continued the study of snake venom cysteine-rich secretory proteins (CRISPs). Snake venom CRISP molecules can cause the paralysis of peripheral smooth muscles and hypothermia by inhibiting certain types of ion channels. The physiological effect of the nose-horned viper CRISPs is still unknown and we intend to describe it.

In 2016 we initiated a Slovenian-Croatian bilateral research project. The result of a common work with colleague immunologists from the University of Zagreb and medical doctors from the Centre for Clinical Toxicology and

Pharmacology, University Medical Centre Ljubljana (UMC) is the publication of two papers. In the first, we described the efficiency of a commercial anti-venom directed towards European viperids (Viperfav™) on a real patient. The key conclusion of this work is that the dose of Viperfav™, recommended for the treatment of persons envenomed by the venom of *Vipera aspis* or *Vipera berus berus*, is probably not enough in the case of a serious envenomation by the venom of *Vipera ammodytes ammodytes* (T. Kurtović et al., *Toxins*, 8 (2016), 244). For this reason, we recommended constant monitoring of such patients during anti-venom treatment. In the second paper, which is accepted for publication (M. Brvar et al., *Clinical Toxicology*, in press), we describe the treatment of patients, envenomed by the nose-horned viper venom, using anti-venom directed towards the common adder venom (ViperaTAB®). We found that the treatment using paraspecific anti-venom alleviated the swelling and temporarily improved the systemic effects of envenomation, by lowering the concentration of toxic components in the patients' blood, but it did not eliminate the neurotoxic effects.

In the past year we also invested a lot of energy in the popularization of our scientific activity by presenting our work to the broader community. Invited by the SATENA society, I. Križaj presented a public lecture in the scope of the action "Science on Street". The lecture entitled "Animal Venoms: from Deadly to the Healthy" was very well attended and received an excellent response (Figure 2). The lecture was recorded and is available at Videlectures.net ([http://videlectures.net/znanostnacesti\\_krizaj\\_zivalski\\_strupi/](http://videlectures.net/znanostnacesti_krizaj_zivalski_strupi/)). Furthermore, we participated at the preparation and presentation of a popular scientific TV broadcast "Bite the Science" entitled "Animal Venoms – Deadly and Useful" (<http://4d.rtvsllo.si/arhiv/ugriznimo-znanost/174441881>). As well, we presented toxinology and our achievements in this field of science in two interviews: for the national radio in an emission "Frequency X" on animal venoms (<http://4d.rtvsllo.si/arhiv/frekvenca-x/174442156>) and for the Slovenian Press Agency (<http://znanost.sta.si/2318140/z-zivalskimi-strupi-do-zdravljenja-bolezni-pri-ljudih>).

#### Lipid metabolism and signalization

Tumours display changes in metabolism that maximize their ability to proliferate and survive during times of stress. Apart from the dependence of many cancer types on glucose and glutamine, lipid metabolism is also altered in cancer. An increased availability of fatty acids (FAs), either through *de novo* synthesis in tumour cells or from exogenous sources, is needed for the synthesis of membranes and signalling molecules that are indispensable for tumour growth, and limiting FA supply may prevent cell proliferation in



Figure 2: Science on the Street on animal venoms. Prof. Igor Križaj during the presentation of a public lecture entitled "Animal Venoms: from Deadly to the Healthy" in Kavarna Union in Ljubljana. The event, attended by more than 200 people, was organized in the scope of the "Science on the Street" project by the Slovenian Academic Society for Science and Engineering (SATENA).

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**Lipid droplets are antioxidant organelles that increase the resistance of cancer cells to stress.**

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tumours. The transformed properties of cancer cells depend on the changes in lipolysis, FA oxidation, membrane phospholipid hydrolysis and reacylation pathways, and the provision of FAs from the circulation. Additionally, the accumulation of neutral lipids in cytosolic lipid droplets has been confirmed in several cancers. Discovering the critical links between cancer-cell survival and lipid metabolism has a strong therapeutic potential.

Lipid droplets are newly recognized organelles composed of a core of neutral lipids, including triacylglycerol and cholesterol esters, and are covered with a phospholipid monolayer and lipid droplet-associated proteins. They are not passive repositories of energy, but act as platforms integrating cellular lipid metabolism and signalling, FA trafficking, protein management and quality control, viral replication and immunity. However, relatively little is known about the role of lipid accumulation and lipid droplets in cancer. sPLA<sub>2</sub>s are lipolytic enzymes that hydrolyse membrane phospholipids and release free FAs and lysophospholipids. sPLA<sub>2</sub> activity leads to the release of a mixture of mono- and polyunsaturated FAs (PUFAs), including omega-6 and omega-3 PUFAs. We have recently reported a novel mechanism of action of sPLA<sub>2</sub> in cancer, describing for the first time a relationship between membrane hydrolysis, lipid droplet formation and breast cancer cell survival. We have found that by inducing lipid droplet formation the sPLA<sub>2</sub> enzyme augments cell proliferation and prevents cell death in breast-cancer cells exposed to nutrient deprivation-induced stress. Our recent, soon to be published, data show that lipid droplets help in reducing oxidative stress as well, particularly in cancer cells exposed to starvation or high levels of oxidation-prone PUFAs in the environment. Furthermore, blocking lipid droplets breakdown by depleting cells of a crucial lipase (Figure 3) led to a reduction in PUFA-induced oxidative stress, suggesting that lipid droplets serve as antioxidant storage depots preventing the damage induced by the easily oxidisable PUFAs. Clearly, lipid droplets are emerging as critical regulators of cancer-cell survival during stress induced by nutrient deprivation and lipotoxic insults, properties which can be exploited to specifically target cancer cells that are known for their high resilience to oxidative and metabolic stress.

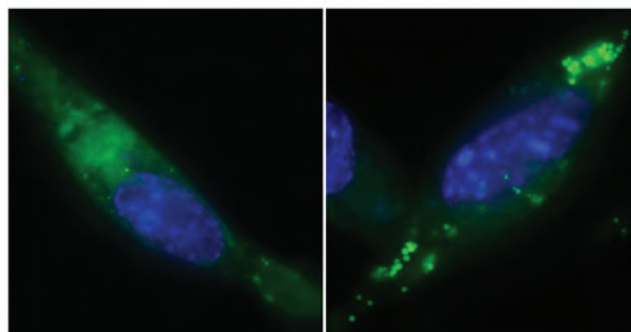


Figure 3: Depleting cells of a lipase involved in lipid droplet breakdown leads to a reduction in lipolysis and a significant increase in the size and number of lipid droplets. Control cells are on the left-hand side and lipase-depleted cells on the right. Lipid droplets were visualized using neutral-lipid specific staining with the BODIPY 493/503 fluorescence dye and nuclei with DAPI. The photographs were acquired using a Zeiss AxioObserver Z1 microscope.

#### High-throughput genetics and functional genomics in yeast *Saccharomyces cerevisiae*

Polygenic trait analysis is one of the fastest-developing fields in genetics. The identification of causal alleles for such traits, which cover the vast majority of all, has almost become routine in model organisms like yeast. The application of this knowledge holds great promise for biomedicine and for biotechnology in the development of new cell factories (J.P. Meijnen et al., *Biotechnol. Biofuels*, 9 (2016), 5). Methods for accurate genome editing that enable the insertion of causal alleles are necessary for the efficient application of such knowledge. To this end, we developed our own protocol of the CRISPR/Cas9 method for genome editing in yeast. This enables us fast and efficient assembly of new combinations of alleles and the generation of strains with the desired traits. We have been using this approach in the development of yeast strains with varying amounts of neutral lipids.

In 2016 we also made important progress in the field of promoter development for the tight regulation of the expression of genes – endogenous and heterologous alike – in yeast cells. Promoters are a key element of the synthetic biology toolbox. We therefore optimized methods for an accurate determination of the strength and variability for the expression of promoter libraries.

A paper was published in 2016 describing the most sophisticated method for large-scale microorganism phenotyping (M. Zackrisson et al., *G3*, 6 (2016), 3003–3014). The core of the method, which is based on unprecedentedly fast and accurate analysis of microorganisms' colony morphology (Figure 4), has been developed at the Jožef Stefan Institute and developed, in collaboration with a group from Sweden, into a key method for polygenic trait analysis.

#### Analysis of genomes

The S1 family of serine peptidases is the largest family of peptidases. Its members are specifically inhibited by Kunitz/BPTI inhibitors. The Kunitz domain is characterized by a compact 3D structure with the most important inhibitory loops for the inhibition of S1 peptidases. In the present study we analysed the action of site-specific positive selection and its impact on the structurally and functionally important parts of the snake venom Kunitz/BPTI family of proteins (V. Župunski & D. Kordiš, *Sci. Rep.*, 6 (2016), 37054). By using numerous models we demonstrated the

#### Polygenic trait analysis in yeast for the development of biomedicine and biotechnology.

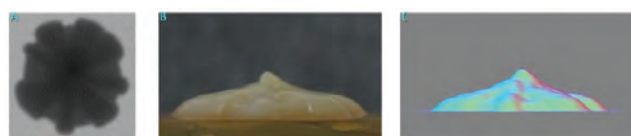


Figure 4: Microorganisms' colony morphology analysis for the Scanomatic method. (A) Transmission scanning of a colony. (B) Side-view portrait of the colony. (C) Computational reconstruction of the colony's morphology.



**Positive selection changes the electrostatic potential on the surface of Kunitz/BPTI proteins that may play an important role in the precise targeting of these inhibitors into the active site of the S1 family of serine peptidases.**

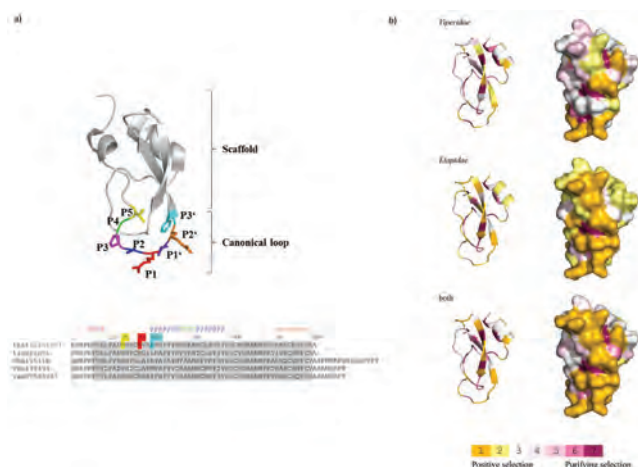


Figure 5: Positively selected amino acids on a three-dimensional model of textilinin-1. a) Structure of textilinin-1 (3BYB) showing the canonical inhibitory loop and protein scaffold. b) Positively selected amino acids in the structure of textilinin-1 (3BYB) are coloured in orange (PP=0.99) and yellow (PP>0.95). The figure is reproduced from V. Župunski & D. Kordiš, *Sci. Rep.*, 6 (2016), 37054.

presence of large numbers of site-specific, positively selected sites that can reach between 30–50% of the Kunitz domain. Mapping of the positively selected sites on a 3D model of Kunitz/BPTI inhibitors has shown that these sites are located in the structurally most important part of the molecule, in the inhibitory loops 1 and 2, and also in the Kunitz scaffold (Figure 5). Amino acid replacements are localized exclusively on the surface, with the vast majority of replacements causing the change of charge. The consequence of these substitutions is the change in electrostatic potential on the surface of Kunitz/BPTI proteins that may play an important role in the precise targeting of these inhibitors into the active site of the S1 family of serine peptidases. The presence of the multigene families of Kunitz/BPTIs in venomous snakes can be explained by the target-oriented arms race, since the number of S1 peptidases in vertebrate preys can reach up to hundreds of representatives. As Kunitz/BPTIs are broad-spectrum inhibitors, they can be functionally diversified to target numerous and diverse S1 peptidases in their prey. A comparison of the Kunitz/BPTI inhibitors from venomous snakes with those from ticks and vampire bats has demonstrated that they experienced strong and widespread action of site-specific positive selection only in venomous snakes.

Antimicrobial peptides (AMPs) are one of the oldest defence components of the innate immune system. Although numerous AMP families are present in prokaryotes and eukaryotes, the greatest diversity can be seen in vertebrates. Since AMPs can inhibit the growth of bacteria, fungi and viruses, they are used in the development of novel antibiotics and immuno-regulatory compounds. The evolution of antimicrobial peptides in vertebrates is still not well explained, mostly because of the confusion in genomic and proteomic databases. A genomic and transcriptomic analysis of all AMP families in vertebrates has been made. In numerous databases we analysed the distribution

of AMP families in vertebrates, from the oldest cyclostomes to the land vertebrates. We demonstrated that besides the numerous lineage-specific AMP families vertebrates also possess a number of common AMP families. We have found that the vertebrate ancestor possessed diverse AMP families that survived hundreds of millions years and that evolutionary younger, lineage-specific AMP families originated several times independently. We have obtained a new insight into the origin, evolution and functional diversification of numerous AMP families in vertebrates.

### Other subjects

In 2016 we also participated at several research projects out of the thematic scope of our department.

Together with our programme group colleagues from the Biotechnical Faculty of the University of Ljubljana (BF UL) we have been analysing the toxin Cdt (cytotoxic distending toxin) from the bacteria *Aggregatibacter actinomycetemcomitans* associated with a severe form of periodontal disease. We also confirmed the existence of a shorter form of the B subunit of this trimeric toxin (CdtB) on the protein level in patients with periodontal disease. This finding may result in new insights into this disease and its treatment (D. Obradović et al., *PLoS One*, 11 (2016), e0159231).

With them, we also analysed the influence of OlyA-mCherry, a fluorescent derivative of ostreolysin A from the mushroom *Pleurotus ostreatus*, on Madin-Darby canine kidney cells. We discovered that by binding on cholesterol- and sphingomyelin-enriched membrane nano-domains the derivative induced formation of vesicles into the extracellular space. At detail characterization of the formed vesicles, potentially interesting model for biophysical and biochemical studies of cell membranes and as a system for non-invasive sampling of cytosol from cells, our task was to analyse their protein composition (M. Skočaj et al., *Biochim. Biophys. Acta - Biomembranes*, 1858 (2016), 2882–2893).

We are partners in the targeted research project (CRP) “Definition of molecular parameters for protection of Carniolan honeybee” that is coordinated by the Zootechnical Department at BF UL. In 2016, we continued a comparative proteomic analysis of haemolymph, royal jelly and venom of the local populations of carniolan honeybee (*Apis mellifera carnica*). In this project we also contributed with a bio-informatic analysis of the collected data. Our results so far have been preliminarily presented (J. Božič et al., *Acta Agricult. Slov.*, Suppl. 5 (2016), 18–27).

For our colleagues from the Medical Faculty of the UL we provided knowledge of the preparation of fluorescently labelled ligands for applications in cell biology. The work describes the internalization of the S100B protein from

the extracellular space into cultured astrocytes and suggests a new way of removing this toxic protein also *in vivo* (E. Lasič et al., *J. Neurochem.*, 139 (2016), 309–323).

For our colleagues from the Department of Nanostructured Materials – K7 at the Jožef Stefan Institute we provided a mass spectrometric analysis of the protein composition of their preparation of fibroin from natural silk, one of the most promising natural materials as a support material in tissue regeneration. A prerequisite for a safe application in human medicine is the preparation of fibroin without a trace of another silk protein sericin due to its high immunogenicity. We succeeded in confirming the perfection of the developed procedure to prepare medically compatible fibroin from the raw silk (N. Drnovšek et al., *J. Mater. Chem. B*, 4 (2016), 6597–6608).

Researchers from the Department of Physical and Organic Chemistry – K3 at the IJS are also interested in the synthesis of new antimalarial substances. Together with them we prepared a review paper about malarial toxins in which we suggested several original strategies directed against this group of toxins (K. Starkl Renar et al., *Toxicon*, 119 (2016), 319–329).

As partners in a project led by colleagues from the Faculty of Electrical Engineering of the UL we accomplished a structural identification analysis of the protein corona composition of nanoparticles prepared in different dispersion media. As the protein corona of nanoparticles primarily determines the pathophysiological characteristics of nanoparticles in biological systems, knowledge about its controlled formation is vitally important for the safe use of nanoparticles in medicine. Our publication reporting about the dependency of the protein corona composition of nanoparticles on the procedure of nanoparticles preparation is in press (K. Strojan et al., *PLoS One*, in press).

### Some outstanding publications in the past year

1. Župunski, V. and Kordiš, D.: Strong and widespread action of site-specific positive selection in the snake venom Kunitz/BPTI protein family. *Sci. Rep.*, 6 (2016), 37054
2. Latinović, Z., Leonardi, A., Šribar, J., Sajevec, T., Žužek, M.C., Frangež, R., Halassy, B., Trampuš-Bakija, A., Pungerčar, J. and Križaj, I.: Venomics of *Vipera berus berus* to explain differences in pathology elicited by *Vipera ammodytes ammodytes* envenomation: Therapeutic implications. *J. Proteomics*, 146 (2016), 34–47
3. Kurtović, T., Brvar, M., Grenc, D., Lang Balija, M., Križaj, I. and Halassy, B.: A single dose of Viperfav™ may be inadequate for *Vipera ammodytes* snake bite: A case report and pharmacokinetic evaluation. *Toxins*, 8 (8) (2016), 244
4. Skočaj, M., Yu, Y., Grundner, M., Resnik, N., Bedina Zavec, A., Leonardi, A., Križaj, I., Guella, G., Maček, P., Erdani-Kreft, M., Frangež, R., Veranič, P. and Sepčić, K.: Characterisation of plasmalemmal shedding of vesicles induced by the cholesterol sphingomyelin binding protein, ostreolysin A-mCherry. *Biochim. Biophys. Acta – Biomembranes*, 1858 (2016), 2882–2893
5. Obradović, D., Gašpersič, R., Caserman, S., Leonardi, A., Jamnik, M., Podlesek, Z., Seme, K., Anderluh, G., Križaj, I., Maček, P. and Butala, M.: A cytolethal distending toxin variant from *Aggregatibacter actinomycetemcomitans* with an aberrant CdtB that lacks the conserved catalytic histidine 160. *PLoS One*, 11 (2016), e0159231

### Organization of conferences and meetings

1. Annual meeting of co-workers of the research programme Toxins and Biomembranes from the Department of Molecular and Biomedical Sciences at the Jožef Stefan Institute and the Department of Biology, Biotechnical Faculty, University of Ljubljana, Ljubljana, 22–23 November 2016
2. 10th Young Researchers' Day (Chemistry, Materials, Biochemistry, Environment), Jožef Stefan Institute, Ljubljana, 31 March 2016

## INTERNATIONAL PROJECTS

1. 7FP - YeSVitE: Yeasts for the Sustainability in Viticulture and Oneology  
Prof. Uroš Petrovič  
European Commission
2. Antivenomics as a Tool to increase Efficacy of Specific and Paraspecific Serotherapy against Envenomation with Viperidae Venoms  
Prof. Igor Križaj  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Toxins and biomembranes  
Prof. Igor Križaj

## R&D GRANTS AND CONTRACTS

1. Thermophoretic guidance, accumulation and sorting of biomolecules in microfluidic devices  
Prof. Igor Križaj
2. Integrative research of sexual dimorphism evolution  
Prof. Dušan Kordiš
3. Applications of aegerolysin-like proteins for detection and eradication of pests  
Prof. Igor Križaj
4. Genetic background of mastitis resistance  
Prof. Igor Križaj
5. Evaluation of possible harmful effects of nanoparticles and underlying mechanisms – from physico-chemical and in vitro toxicity characterisation to innate immune system activation  
Prof. Igor Križaj
6. Crosstalk between lipid and central carbon metabolism  
Prof. Uroš Petrovič

7. Bisphenol A alternatives: transfer from food contact material, fate and human exposure  
Asst. Prof. Toni Petan
8. Improved treatment and monitoring of Water Framework Directive priority pollutants  
Prof. Igor Križaj

9. Definition of molecular parameters for protection of Carniolan honeybee  
Prof. Igor Križaj

## VISITORS FROM ABROAD

1. Federica Valdetara, University of Milan, Milan, Italy, 16 January – 18 March 2016 and 1–16 July 2016
2. Dr Beata Halassy, Centre for Research and Knowledge Transfer in Biotechnology, University of Zagreb, Zagreb, Croatia, 8 June 2016
3. Dr Tihana Kurtović, Centre for Research and Knowledge Transfer in Biotechnology, University of Zagreb, Zagreb, Croatia, 8 June 2016
4. Dr Maja Lang Balija, Centre for Research and Knowledge Transfer in Biotechnology, University of Zagreb, Zagreb, Croatia, 8 June 2016
5. Merve Yilmazer, University of Istanbul, Istanbul, Turkey, 19 October 2016 – 17 February 2017

## 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. Asst. Prof. Toni Petan
  7. Dr. Jernej Šribar
- Postgraduates**
8. Eva Jarc, B. Sc.
  9. *Minca Klobčar, B. Sc., left 15.08.16*

10. Mojca Ogrizović, B. Sc.
  11. Sabina Ott, B. Sc.
- Technical officers**
12. *Miha Škalič, B. Sc., left 07.06.16*
- Technical and administrative staff**
13. Igor Koprivec
  14. Maja Šimaga, M. Sc.
  15. *Darja Zunič Kotar, retired 01.06.16*

Note:

\* part-time JSI member

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### ORIGINAL ARTICLE

1. Nataša Drnovšek, Rok Kocen, Ana Gantar, Marinka Drobnič-Košorok, Adrijana Leonardi, Igor Križaj, Aleksander Rečnik, Saša Novak, "Size of silk fibroin  $\beta$ -sheet domains affected by  $Ca^{2+}$ ", *J. mater. chem. B*, vol. 4, iss. 40, pp. 6597-6608, 2016.
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5. Zorica Latinović, Adrijana Leonardi, Jernej Šribar, Tamara Sajevec, Monika C. Žužek, Robert Frangež, Beata Halassy, Alenka Trampuš-Bakija, Jože Pungerčar, Igor Križaj, "Venomics of *Vipera berus berus* to explain differences in pathology elicited by *Vipera ammodytes ammodytes* envenomation: Therapeutic implications", *Journal of proteomics*, vol. 146, pp. 34-47, 2016.
6. Jean-Paul Meijnen, Paola Randazzo, María R. Foulquié-Moreno, Joost van den Brink, Paul Vandecruys, Marija Stojiljkovic, Françoise Dumortier, Polona Zalar, Teun Boekhout, Nina Gunde-Cimerman, Janez Kokošar, Miha Štajdohar, Tomaž Curk, Uroš Petrovič, Johan M. Thevelein, "Polygenic analysis and targeted improvement of the complex trait of high acetic acid tolerance in the yeast *Saccharomyces cerevisiae*", *Biotechnol. biofuels*, vol. 9, pp. 1-18, 2016.
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8. Matej Skočaj, Yang Yu, Maja Grundner, Nataša Resnik, Apolonija Bedina Zavec, Adrijana Leonardi, Igor Križaj, Graziano Guella, Peter Maček, Mateja Erdani-Kreft, Robert Frangež, Peter Veranič, Kristina Sepčič, "Characterisation of plasmalemmal shedding of vesicles induced by the cholesterol/ sphingomyelin binding protein, ostreolysin A-mCherry",

*Biochim. biophys. acta, Biomembr.*, vol. 1858, no. 11, pp. 2882-2893, 2016.

9. Martin Zackrisson *et al.* (14 authors), "Scan-o-matic: High-resolution microbial phenomics at a massive scale", *G3 (Bethesda Md.)*, vol. 6, no. 9, pp. 3003-3014, 2016.
10. Vera Župunski, Dušan Kordiš, "Strong and widespread action of site-specific positive selection in the snake venom Kunitz/BPTI protein family", *Scientific reports*, vol. 6, pp. 37054-1-37054-12, 2016.

### REVIEW ARTICLE

1. Katarina Starkl, Jernej Iskra, Igor Križaj, "Understanding malarial toxins", *Toxicol (Oxford)*, vol. 119, pp. 319-329, 2016.

### PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

1. Janko Božič, Dušan Kordiš, Igor Križaj, Adrijana Leonardi, Robert Močnik, Mitja Nakrst, Peter Podgoršek, Janez Prešern, Simona Sušnik Bajec, Minja Zorc, Jelena Zorc, Peter Dovč, "Novel aspects in characterisation of Carniolan honey bee (*Apis mellifera carnica*, Pollmann 1879)", In: *Technology driven animal production*, (Acta agriculturae slovenica, Supplement, 2016, 5), 24th International Symposium Animal Science Days, Ptuj, September 21st-23rd, 2016, pp. 18-25.

### UNIVERSITY, HIGHER EDUCATION OR HIGHER VOCATIONAL EDUCATION TEXTBOOK

1. Nataša Debeljak, Simon Horvat, Peter Juvan, Rok Košir, Tanja Kunej, Uroš Petrovič, Tadeja Režen, Damjana Rozman, Jure Ačimovič (urednik), *Funkcijska genomika: praktikum*, 2. izd., Ljubljana, Medicinska fakulteta, 2016.

### MENTORING

1. Urša Kresal, *Metabolism and transport of fatty acids in the action of secreted phospholipases A<sub>2</sub> in breast cancer cells*: master's thesis, Ljubljana, 2016 (mentor Jože Pungerčar; co-mentor Toni Petan).
2. Petra Malavašič, *Phospholipases A<sub>2</sub> and changes in the synthesis, storage and use of lipids in cancer cells*: master's thesis, Ljubljana, 2016 (mentor Igor Križaj).

# DEPARTMENT OF BIOTECHNOLOGY

## B-3

*At the Department of Biotechnology we investigate the 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 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 in the search for new biotechnological approaches and products.*



Head:  
**Prof. Janko Kos**

As in previous years, also in 2016, we studied the structure and function of various fungal enzymes, inhibitors and lectins. Mushrooms represent a promising source of bioactive proteins and biopesticides based on their own arsenal of various compounds used against pests, parasites and pathogens. Among them, defense proteins are very important and include lectins and protease inhibitors with strong and specific insecticidal and/or nematocidal activity. Phylogenetic analyses revealed that these proteins are widely present among higher fungi, ascomycetes and basidiomycetes. These protein toxins have potential applications in veterinary and human medicine and in crop protection. We have also described the medicinal properties of mushrooms belonging to the genus of funnel mushrooms (*Clitocybe* sp.) and of lectins from clouded funnel (*Clitocybe nebularis*), which show antitumor, immunomodulatory, antioxidative and antimicrobial (antiviral, antibacterial, and antifungal) activities.

The search for novel antibacterial compounds from mushrooms in cooperation with the National Institute of Biology using the plant pathogenic bacterium *Ralstonia solanacearum* as the model led to isolation and characterization of the protein complex with L-amino acid oxidase activity. Interestingly, these enzymes with antibacterial activity that were previously described mainly as major components of snake venoms, are also present in poisonous mushrooms such as the death cap (*Amanita phalloides*) and surprisingly also in edible mushrooms such as the trooping funnel (*Clitocybe geotropa*).

The continuing study on the involvement of proteases in plant response to drought showed a new level of complexity demonstrating that different stages of water deficit correlate to different levels of peptidase activities in leaves of different ages in common bean plants.

The studies in the field of glycobiology in 2016 focused on lectins from different mushrooms and their effects on different cell lines, with emphasis on immune cells. We confirmed the exclusive cytotoxicity of CNL lectin from clouded funnel against leukemic T cells Jurkat causing programmed cell death through binding a receptor in a plasma membrane.

Investigating the role of proteolytic enzymes in the regulation of cell cytotoxicity we focused our work on cathepsins C and H, two main convertases of progranzyme B, the molecule which triggers the processes of cell death. The activity of cathepsins C and H in secretory vesicles is controlled by the endogenous inhibitor cystatin F. Using different cystatin F mutants we analyzed the mechanism of its secretion, activation and cell uptake on different cell lines. With different cystatin F mutants we identified its target proteases involved in the regulation of the cytotoxicity of natural killer cells (NK cells) and confirmed its involvement in the reduced cytotoxicity of anergized NK cells. To study the involvement of cystatin F in the regulation of cytotoxic T lymphocyte function we established a model of cytotoxic T lymphocytes with reduced cytotoxicity. Using this model we can further study mechanisms leading to lower cytotoxicity after the interaction of cytotoxic cells with tumor cells. We found increased cystatin F levels in cells with lower cytotoxicity. Furthermore, using antibodies against LAMP1 and flow cytometric analysis we confirmed that exocytosis is not blocked in these cells.

In the field of neurobiology we published three articles in reputable journals on the topic of molecular processes underlying frontotemporal dementia (FTD) and amyotrophic lateral sclerosis (ALS). In our most acclaimed publication and in collaboration with a large international consortium

- **New genes associated with amyotrophic lateral sclerosis were discovered**
- **The aggregation of TDP-43 leads to the loss of its function**
- **The current understanding of the role of nuclear transport in ALS and FTD was critically reviewed**



Figure 1: Death cap is a source of various bioactive compounds including antibiotics and trypsin inhibitors.

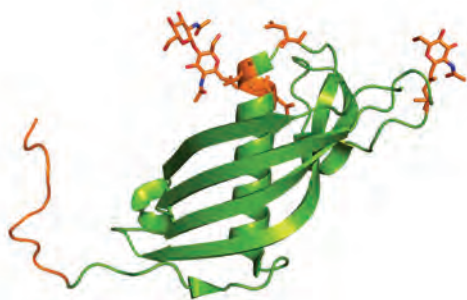


Figure 2: Ribbon diagram of human cystatin F with mutants indicated in orange.

- **L-amino-acid oxidases from Amanita phalloides and Clitocybe geotropa induce caspase-dependent apoptosis**
- **The functional recombinant B subunit of shiga toxin, Stx1B was produced and expressed on the surface of lactic acid bacterium Lactococcus lactis**

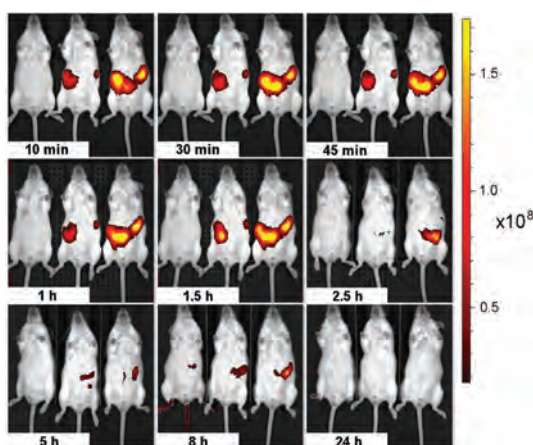
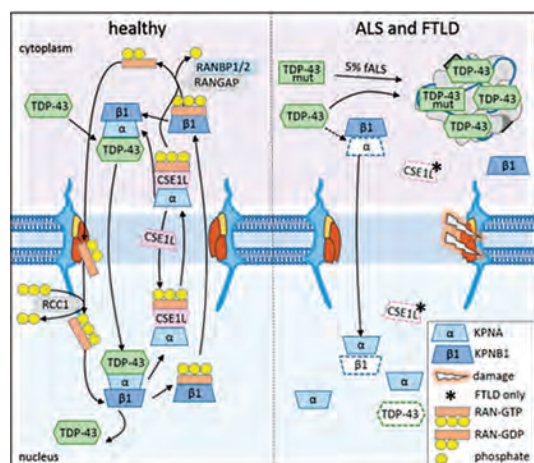


Figure 3: Representative example of 24h time-course imaging of mice administered with no bacteria (left; control),  $2.5 \times 10^{10}$  cells of IRFP713-expressing *L. lactis* (middle) and  $5.0 \times 10^{10}$  cells of IRFP713-expressing *L. lactis* (right). Colour bar indicates radiant efficiency.



we reported new genes and gene regions that are associated with the development of ALS. The study was published in the journal *Nature Genetics* and has received a substantial response in foreign and domestic media. Upon publication, we had several television, radio and newspaper interviews and reports. In the second article, we focused on the impact of the lack of protein TDP-43 on cell proteome (Prpar Mihevc et al., *Scientific Reports*). In cooperation with a group of ICGEB, Trieste, we found that the aggregation of TDP-43 leads to a similar lack of specific proteins as silencing or loss of TDP-43. We also published a review article in the prestigious journal *Brain*, on the nuclear transport in ALS (Prpar Mihevc et al., *Brain*).

Infections with shiga toxin-producing bacteria, like enterohemorrhagic *Escherichia coli* and *Shigella dysenteriae*, represent a serious medical problem. No specific and effective treatment is available for patients with these infections, creating a need for the development of new therapies. We have produced functional recombinant B subunit of shiga toxin, Stx1B, in *Escherichia coli* and used it as a target for the selection of ABD variants from the ABD scaffold-derived high-complex combinatorial library in collaboration with our Czech partners. We have selected 17 different ABD variants (named S1B) with a five-round ribosome display. The two most promising S1Bs (S1B22 and S1B26) were characterized into more details by ELISA, surface plasmon resonance and microscale thermophoresis. The binding affinity to Stx1B was determined to be in the  $1\text{-}\mu\text{M}$  range with both methods. The addition of S1Bs changed the subcellular distribution of Stx1B in HeLa cells, completely eliminating it from Golgi apparatus, most likely by interfering with its retrograde transport. All S1Bs were successfully displayed on the surface of safe lactic acid bacterium *Lactococcus lactis* by fusing to the Usp45 secretion signal and to the peptidoglycan-binding C terminus of AcmA. Binding of Stx1B by engineered lactococcal cells was confirmed using flow cytometry and whole-cell ELISA. Engineered lactic acid bacteria are potentially useful for the removal of Shiga toxin from human intestine. Additionally, novel ABD scaffold-derived Stx1B binders are useful for basic research on Shiga toxin-related infections and could be further improved for in-vitro diagnostics.

The results of the research work at the Department of Biotechnology in the year 2016 were published in 24 scientific papers in journals with an impact factor and in one book chapter. Also, three patent applications were filed. We received two research grants and Ph.D. grant from the Slovenian Research Agency, two bilateral international grants and as partners EU project 'Carbohydrate Metrology', CSA - Coordination & Support Action, Horizon 2020. Two Ph.D. students defended their doctoral theses. Ph.D. Young researcher Ana Bajc Česnik ended a one-year visit to the laboratory of Prof. dr. Cleveland, UCSD, USA. Head of department prof. Janko Kos was elected as a member of European Academy of Sciences and Arts. The members of the department were also very active in pedagogical work as lecturers and mentors to students preparing diploma and doctoral thesis at universities in Slovenia and abroad.

### Some outstanding publications in the past year

1. Prpar Mihevc, Sonja, Darovic, Simona, Kovanda, Anja, Bajc Česnik, Ana, Župunski, Vera, Rogelj, Boris. Nuclear trafficking in amyotrophic lateral sclerosis and frontotemporal lobar degeneration. *Brain*, ISSN 0006-8950, [in press] 2016, 14 str., doi: 10.1093/brain/aww197. COBISS.SI-ID 29663527, IF 10,1.
2. Rheenen, Wouter Van, Shatunov, Aleksey, Dekker, Annelot M., McLaughlin, Russell L., Diekstra, Frank P., Pulit, Sara L., Van Der Spek, Rick A. A., Vösa, Urmo, De Jong, Simone, Robinson, Matthew R., Rogelj, Boris, Vrabec, Katarina, Ravnik-Glavač, Metka, Koritnik, Blaž, Zidar, Janez, Leonardis, Lea, Dolenc-Grošelj, Leja, et al. Genome-wide association analyses identify new risk variants and the genetic architecture of amyotrophic lateral sclerosis. *Nature genetics*, vol. 48, no. 9, str. 1043-1048. [COBISS.SI-ID 3106220], IF 31,6

Figure 4. Model of nuclear transport of TDP-43 in healthy individuals, and in cases of ALS-TDP and FTLD-TDP. TDP-43 is translocated into the nucleus by the classical import pathway. In cases of ALS-TDP and FTLD-TDP TDP-43 is mislocalized to cytoplasmic inclusions. Reduced levels of CSE1L in FTLD-TDP and loss of nuclear KPNA in ALS-TDP imply that this is due to nuclear transport defect. Proteins with reduced levels are in dashed brackets. From Prpar Mihevc et al., *Brain* 2016).

3. McKinnon, Brett D., Kocbek, Vida, Nirgianakis, Kostantinos, Bersinger, Nick A., Mueller, Michael D. Kinase signalling pathways in endometriosis : potential targets for non-hormonal therapeutics. Human reproduction update, ISSN 1355-4786, [in press] 2016, 22 str., doi: 10.1093/humupd/dmv060. [COBISS. SI-ID 29436455], IF 11,2

## Organization of conferences and meetings

1. 10<sup>th</sup> Young researchers' day (Chemistry, Materials, Biochemistry, Environment), Jožef Stefan Institute, Ljubljana, 31 March 2016
2. Day of Biomolecular Sciences – Biomolekularec 2016, Faculty of Medicine, University of Ljubljana, Ljubljana, 22 September 2016
3. Annual meeting of co-workers of the research programme Pharmaceutical Biotechnology: Knowledge for Health, from the Department of Biotechnology at the Jožef Stefan Institute and the, Chair of Pharmaceutical Biology, Faculty of Pharmacy, University of Ljubljana, 1 December 2016

## Patent granted

1. Tadej Rejc, Uroš Petrič, Jana Debeljak, Toni Bremec, Polonca Ferk, Mojca Lunder, Irena Roškar, Borut Štrukelj, Samo Kreft, Mixture of natural polyphenols from white fir wood for reducing postprandial glucose concentration, SI24984 (A), Slovenian Intellectual Property Office , 30. 11. 2016.

## INTERNATIONAL PROJECTS

1. Functional and Structural Studies of Lectins from Mushrooms  
Dr. Jerica Sabotič  
Slovenian Research Agency
2. The Role of C/EBP Alpha in Regulation of Cystatin F Expression  
Prof. Janko Kos  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Pharmaceutical Biotechnology: Knowledge for Health  
Prof. Janko Kos

## R & D GRANTS AND CONTRACTS

1. Dysregulation of TDP-43 expression in amyotrophic lateral sclerosis and frontotemporal lobar degeneration  
Prof. Boris Rogelj
2. Nitroxoline and its derivatives as new antitumour drugs  
Dr. Janko Kos
3. Post-transcriptional regulatory networks in neurodegenerative diseases  
Prof. Boris Rogelj
4. Genetics and pharmacogenomics of inflammatory bowel diseases and genetically related chronic immune diseases  
Prof. Boris Rogelj
5. Pathogenic mechanism of the C9orf72 expanded hexanucleotide repeat mutation in neurodegeneration  
Prof. Boris Rogelj
6. The role of cysteine protease inhibitors in NK cell mediated lysis of tumour cells  
Prof. Janko Kos
7. Protein engineering of recombinant probiotic lactic acid bacteria for treatment of irritative bowel disease  
Prof. Borut Štrukelj

## VISITORS FROM ABROAD

1. Dr. Tibor Hortobagy, University of Debrecen, Debrecen, Hungary, 24 May – 25 May 2016
2. Prof. Daniel H. Wreschner, University of Tel Aviv, Tel Aviv, Israel, 4 July 2016
3. Dr. Adeleta Softić, Faculty of Pharmacy, University of Tuzla, Tuzla, Bosnia and Herzegovina, 21 August – 31 August 2016
4. Esmeralda Dautović, M.Sc., Faculty of Pharmacy, University of Tuzla, Tuzla, Bosnia and Herzegovina, 21 August – 22 November 2016

## STAFF

### Researchers

1. Asst. Prof. Aleš Berlec
  2. Prof. Janko Kos\*, Head
  3. Prof. Boris Rogelj
  4. Dr. Jerica Sabotič
  5. Prof. Borut Štrukelj\*
- ### Postdoctoral associates
6. Dr. Vida Kocbek
  7. Dr. Špela Konjar
  8. Dr. Anja Kovanda
  9. Dr. Milica Perišić Nanut
  10. Dr. Sonja Prpar Mihevc
  11. Dr. Anja Pucer Janež

12. Dr. Petra Zadravec, left 01.08.16

### Postgraduates

13. Ana Bajc Česnik, B. Sc.
14. Dr. Simona Darovic, left 01.06.16
15. Mirjana Malnar, B. Sc.
16. Mateja Prunk, B. Sc.
17. Katja Škrlec, B. Sc.

### Technical and administrative staff

18. Maja Šimaga, M. Sc.
19. Darja Žunič Kotar, retired 01.06.16

Note:

\* part-time JSI member

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## ORIGINAL ARTICLE

1. Maruška Budič, Blaž Cigić, Maja Šoštarčič, Jerica Sabotič, Vladimir Meglič, Janko Kos, Marjetka Kidrič, "The response of aminopeptidases of *Phaseolus vulgaris* to drought depends on the developmental stage of the leaves", *Plant physiol. biochem. (Paris)*, vol. 109, pp. 326-336, 2016.
2. Jana Debeljak, Polonca Ferik, Miro Čokolič, Andrej Zavratnik, Eva Tavčar Benkovič, Samo Kreft, Borut Štrukelj, "Randomised, double blind, crossover, placebo and active controlled human pharmacodynamic study on the influence of silver fir wood extract (Belinal) on post-prandial glycaemic response", *Pharmazie*, vol. 71, no. 10, pp. 566-569, 2016.
3. Gorazd Drevenšek, Mojca Lunder, Eva Tavčar Benkovič, Borut Štrukelj, Samo Kreft, "Cardioprotective effects of silver fir (*Abies alba*) extract in ischemic-reperfused isolated rat hearts", *Food & nutrition research*, vol. 60, pp. 1-7, oct. 2016.
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5. Giovanni Grandi, Michael D. Mueller, Andrea Papadia, Vida Kocbek, Nick A. Bersinger, Felice Petraglia, Angelo Cagnacci, Brett D. McKinnon, "Inflammation influences steroid hormone receptors targeted by progestins in endometrial stromal cells from women with endometriosis", *J. reprod. immunol.*, vol. 117, pp. 30-38, 2016.
6. Vida Kocbek, Giovanni Grandi, Fabian Blank, Carlos Wotzkow, Nick A. Bersinger, Michael D. Mueller, Satoru Kyo, Brett D. McKinnon, "TNF $\alpha$ -induced IKK $\beta$  complex activation influences epithelial, but not stromal cell survival in endometriosis", *Mol. hum. reprod.*, vol. 22, no. 11, pp. 768-777, 2016.
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8. Jernej Luzar, Peter Molek, Mira Šilar, Peter Korošec, Mitja Košnik, Borut Štrukelj, Mojca Lunder, "Identification and characterization of major cat allergen Fel d 1 mimotopes on filamentous phage carriers", *Mol. immunol.*, vol. 71, pp. 176-183, Mar. 2016.
9. Brett D. McKinnon, Vida Kocbek, Kostantinos Nirgianakis, Nick A. Bersinger, Michael D. Mueller, "Kinase signalling pathways in endometriosis: potential targets for non-hormonal therapeutics", *Hum. reprod. updat.*, vol. 22, no. 3, pp. 382-403, 2016.
10. Ana Mitrovič, Jakob Kljun, Izidor Sosič, Stanislav Gobec, Iztok Turel, Janko Kos, "Clioquinol-ruthenium complex impairs tumour cell invasion by inhibiting cathepsin B activity", *Dalton trans. (2003)*, vol. 45, iss. 42, pp. 16913-16921, 2016.
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2. Jure Pohleven, Janko Kos, Jerica Sabotič, "Medicinal properties of the genus *Clitocybe* and of lectins from the clouded funnel cap mushroom, *C. nebularis* (Agaricomycetes): a review", *Int. j. medic. mushrooms*, vol. 18, no. 11, pp. 965-975, 2106.
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4. Jerica Sabotič, Robin Ohm, Markus Künzler, "Entomotoxic and nematotoxic lectins and protease inhibitors from fungal fruiting bodies", *Appl. microbiol. biotechnol.*, vol. 100, no. 1, pp. 91-111, 2016.
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Jerica Sabotič, Janko Kos, "Fungal protease inhibitors", In: *Fungal metabolites*, (Reference Series in Phytochemistry), J. M. Merillon, ed., K. G. Ramawat, ed., Berlin, Springer, 2016, 33 pp.

## PATENT

1. Tadej Rejc, Uroš Petrič, Jana Debeljak, Toni Bremec, Polonca Ferik, Mojca Lunder, Irena Roškar, Borut Štrukelj, Samo Kreft, *Mixture of natural polyphenols from white fir wood for reducing postprandial glucose concentration*, SI24984 (A), Urad RS za intelektualno lastnino, 30. 11. 2016.

## MENTORING

1. Simona Darovic, *Modifications of FUS and implications in pathological changes in neurodegenerative diseases*: doctoral dissertation, Ljubljana, 2016 (mentor Boris Rogelj).
2. Petra Zadravec, *Development of genetically modified lactic acid bacteria with shiga toxin binding ability*: doctoral dissertation, Ljubljana, 2016 (mentor Aleš Berlec).

3. Valter Bergant, *Characterization of heterogeneous nuclear ribonucleoprotein H in cytoplasmic stress granules*: master's thesis, Ljubljana, 2016 (mentor Boris Rogelj).
4. Melisa Fazlić, *The function and localization of gamma-enolase in colon cancer Caco-2 cell line*: master's thesis, Ljubljana, 2016 (mentor Janko Kos; co-mentor Tjaša Vižin).
5. Tanja Jakoš, *Novel inhibitors of cysteine peptidase cathepsin X*: master's thesis, Ljubljana, 2016 (mentor Janko Kos; co-mentor Urša Pečar Fonović).
6. Božena Kesić, *Isolation and characterization of cystatin F mutants*: master's thesis, Ljubljana, 2016 (mentor Janko Kos; co-mentor Milica Perišić Nanut).
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11. Klara Tereza Novoselc, *Expression changes in selected proteins after muscle inactivity*: master's thesis, Ljubljana, 2016 (mentor Boris Rogelj; co-mentor Anja Kovanda).
12. Maja Oven, *Evaluation of L-amino acid oxidases as inducers of apoptosis*: master's thesis, Ljubljana, 2016 (mentor Janko Kos; co-mentor Anja Pišlar).





# DEPARTMENT OF ENVIRONMENTAL SCIENCES

## O-2

*The research of the Department of Environmental Sciences deals with fundamental scientific questions about natural environmental systems and processes at various scales, their interactions and responses to human activities, and with the development of technical solutions for environmental problems and environmental management issues. Our research is inter- and multidisciplinary: Environmental analytical chemistry, Biogeochemical cycles, Microbial ecology, Environment and health, Environmental technologies, Risk and environmental assessment, and Environmental monitoring.*

*The department hosts the "ISO-FOOD" ERA Chair for isotope techniques in food safety, quality and traceability, the infrastructure Centre of Mass Spectrometry (CMS) and the Mobile Ecological Laboratory Unit (ELMU).*

### Environmental analytical chemistry

In the field of elemental speciation, a review of monolithic chromatography in the speciation analysis of metal-containing biomolecules has been published, highlighting the great potential of monolithic columns for applications in metallomics. A book chapter was also written on analytical procedures for the speciation of chromium, aluminium and tin in environmental and biological samples.

A procedure has been developed for the quantification of **tributyltin** (TBT) in natural waters at the environmental quality standard level required by the water framework directive. An inter-laboratory comparison of data on TBT determination in whole water samples has also been performed.

A simple analytical method with minimal sample preparation steps was developed for sensitive and reliable determinations of the six PBDEs in sewage sludge by the use of gas chromatography coupled to inductively coupled plasma mass spectrometry (GC-ICP-MS).

In the vast majority of the sample digestion methods the solid residue (silicates, zirconium, etc.) remains undissolved, yielding possible errors in radionuclide determination. A novel methodology for fast sample digestion using lithium borate fusion was developed and applied for the determination of actinides in solid samples. The methodology allows for the complete digestion of solid samples with no residues left, which ensures reliable determinations of the actinides in sample matrices that are difficult to digest.

Following the acquisition of Nu Plasma II multicollector inductively coupled plasma mass spectrometer (MC-ICP-MS), methodologies for the determination of Hg, Pb, Sr and U isotope ratios in various environmental and biological matrices were developed. The application of isotope ratio analysis to environmental studies complements the information on the concentration and speciation of specific elements in the environment and represents a powerful tool in different applications such as tracing the fate of the contaminant in the environment, its biogeochemical transformations or for tracing the origin of food samples.

In the field of the analysis of organic compounds, the group has continued with its research into the fate of pharmaceutical and personal care products and industrial compounds with an endocrine-disrupting effect in environmental and wastewater samples with an emphasis on advanced sampling/extraction. We have developed and published a series of analytical procedures for determining cytostatics (Cyclophosphamide, Ifosfamide, Methotrexate, Imatinib, Vincristin and Etoposide) and their commercially available metabolites in waste and environmental water samples. We showed the presence of detectable quantities of these compounds in wastewaters from hospitals, where cancer therapies are being conducted, in wastewater treatment plant (WWTP) influents and in some effluents. None of the studied cytostatics were detected in receiving waters. Using a newly developed and validated analytical method, we determined the cytostatic bleomycine in serum and tumour tissue in mice and oncologic patients, which were provided by the Institute of Oncology in Ljubljana. The results of these studies were published in international journals with a high impact factor.

Besides cytostatic drugs, also analytical methods for **sertraline** and its metabolites/transformation products norsertraline, sertraline ketone and sertraline imine were developed. To improve the performance of sertraline analysis, we have been developing and testing **molecularly imprinted polymers** (MIPs) with sertraline as the target compound (in collaboration with the Faculty of Chemistry and Chemical Engineering at the University of Maribor). We focused on the problem of sertraline leaching out of the template used during synthesis and choosing the MIP with the highest MIP effect for norsertraline. In the area of industrial chemicals, we developed and



Head:

**Prof. Milena Horvat**

validated analytical methods for the presence of BPA and its alternatives in potable and waste waters and food and food-contact material (FCM) samples (honey). In the case of honey and wastewaters, the analytical method was also applied to a series of honey, FCM and wastewater samples. In addition, we developed an analytical method for determining **diclofenac and other estrogens** listed on the WFD watch list using disk-based solid-phase extraction and GC-MS with the aim of achieving WFD required LOQs and developing a multiresidual analytical method for the simultaneous determination of 48 various compounds of emerging concern (pharmaceuticals, UV filters, preservatives, industrial chemicals etc.). Both validated analytical methods were applied to a series of environmental and wastewater samples.

In the area of **non-target analysis**, we continued with the identification of transformation products of cytostatics (Cyclophosphamide, Ifosfamide, Methotrexate) and identified numerous transformation products for the first time using advanced instrumentation like the LTQ Orbitrap XL mass spectrometer (Curtin University, Perth, Australia; CSIC, Barcelona, Spain). In addition, batch biotransformation experiments of the **antidepressants sertraline and bupropion, antimitotic ketoconazole and three bisphenols (bisphenol Z, S and C2)** was carried out and non-target analyses of their transformation products are currently being evaluated in collaboration with the University of Antwerp, Belgium and EAWAG, Switzerland. In collaboration with the Faculty of Chemistry and Chemical Engineering at the University of Ljubljana, several of the identified transformation products were also synthesised and applied as standards in our research.

Within the Empire project Metra we developed a method for the quantitative determination of elemental mercury in broken fluorescent lamps. We have also developed a method for the determination of MeHg based on derivatization using dithizone and their separation on a chromatographic column and final quantification by using cold vapour atomic fluorescence spectrophotometry.

In the context of the key intercomparison K-127 "Contaminants and other elements in the soil" organized in collaboration with CENAM from Mexico, data were collected and processed in the final report prepared. We participate in the key comparison (KC) CCQM-K140: Carbon Stable Isotope Ratio Delta Values in Honey and in inter-laboratory comparison in food: FIT-PTS, which is organized three times per year by EUROFINS. A group training entitled: "**Metrology in isotope ratio measurements: traceability, uncertainty and comparability**", was organized within the MASSTWIN project in collaboration with Fondazione Edmund Mach (FEM). In total, 44 participants attended the training, representing nine different countries. In the field of metrology the new PRO-METROFOOD project was accepted in order to provide catalytic and leveraging support for the preparatory phase and the early phase of the ESFRI project METROFOOD, leading to the construction of new research infrastructures in the field of food quality, safety and traceability. We also participated in several interlaboratory comparisons organised by WEPAL, IAEA, NPL, BFS, GEOTRACES and MRI.

### Biogeochemical cycles

In the field of **water cycle** investigations, a new Slovenian-Hungarian research project started on the spatial distribution of water isotopes in precipitation on the transect from the Adriatic to the Pannonian Plain. A gap analysis was performed on existing data, to improve the monitoring in the frame of Slovenian Network of Isotopes in Precipitation (SLONIP). The observation network was extended with 6 new stations in the framework of the common research project with the Faculty of Civil and Geodetic Engineering of the University of Ljubljana on the modelling of the hydrologic response of the non-homogeneous Ljubljana river catchment. The SLONIP observation sites will provide input data for on-going and future research of water resources and their management, food authentication, etc.

In the frame of several national and international research projects we continued **isotopic hydrogeochemical research of Slovenian rivers** (Sava, Krka, Pesnica, Radovna and Savica) and groundwater in carbonate fractured aquifers in central Slovenia. Stable isotopes were used as tracers to assess the biogeochemical cycling of nutrients, groundwater recharge and the relation between land use and the quality of ground/surface water. In collaboration with researchers from the Ruder Bošković Institute (Croatia) we participated in studies of the hydrological dynamics of karst springs in Trabaque valley (Spain) from isotopic records of the river and recent and ancient tufa. A hydrological model of overflow springs was generated and a tufa  $\delta^{18}\text{O}$  record under constrained parameters was simulated. The authigenic precipitation of carbonate and pyrite was studied in the lake Kutina, a karstic crypto depression in the Neretva river delta (Croatia) using isotopic methods and field-emission scanning electron microscopy, where the environmental conditions and early diagenetic processes were correlated with the habitus of precipitated phases.

An interpolation model of the spatial distribution of coalbed gas in relation to the structure of the Velenje coal basin was developed, based on data on coalbed gas ( $\text{CO}_2$ ,  $\text{CH}_4$ ) concentrations, their isotopic composition and the Carbon Dioxide Index (CDMI) collected from a 500-m-deep excavation field in collaboration with the Velenje Coalmine d.d. since 2000

A method was developed for **Hg isotope ratio analysis** using MC-ICP-MS, Hg isotopic compositions and evaluation of Hg the isotopic fractionation of soil cores and different ores from the Idrija mercury mine, processed (retorted) ore, native elemental Hg<sup>0</sup><sub>(L)</sub> present in the mine and appearing in the near-by Idrijca river, and elemental Hg<sup>0</sup>, produced in Idrija smelting plant. Preliminary results showed a very variable Hg isotopic composition among the analysed samples, indicating a rich history of biogeochemical transformations of Hg in Idrija.

The research performed within the **GLOBAQUA** project is focused on the Sava River basin (SRB) and comprised: (1) a determination of the sources and mean residence time in the groundwater of Ljubljansko polje aquifer, which represents the main drinking-water supply for Ljubljana and its surroundings using  $\delta^2\text{H}$ ,  $\delta^{18}\text{O}$  and  $^3\text{H}$  and  $^3\text{H}/^3\text{He}$ , respectively; (2) a determination of the sources of nitrate pollution in the Sava River; and (3) modelling the surface-groundwater interactions in the Ljubljansko Polje aquifer. The important upper boundary conditions of the hydrogeological model were determined, describing the spatio-temporal variability of infiltration pathways from the two main groundwater sources: the Sava River and spatial percolation from precipitation and snowmelt. The MIKE 11 and WaSiM software were applied for these purposes and combined with the FEFLOW software for groundwater flow modelling. The use of stable isotopes in hydrological and climate studies was also the subject of the GLOBAQUA training programme organized at the JSI in October 2017.

Further investigations of the **CO<sub>2</sub> fluxes above the subterranean cave** were carried out. Results indicate that the main parameter affecting the ventilation in the investigated cave is the difference between the cave and outside-air temperatures, causing summer stagnation with CO<sub>2</sub> build-up and winter ventilation. The results of stable isotope analysis indicate that the cave CO<sub>2</sub> is a mixture of atmospheric air CO<sub>2</sub> and CO<sub>2</sub> originating from organic matter produced by C3 vegetation. During the cold season, we were able to detect the cave CO<sub>2</sub> influence in soil and estimate its contribution to be up to 80% of soil air CO<sub>2</sub>.

The use of stable isotopes in carbon and CO<sub>2</sub> also has an applied value in other fields of research, for example, for **detecting CO<sub>2</sub> leakage** from proposed subsea carbon capture and storage (CCS) sites, i.e., usually depleted gas and oil reservoirs or saline formations, which lie below the seabed. CCS is regarded as one of the most important long-term measures for reducing carbon globally. In collaboration with the Institute Nazionale di Oceanografia e Geofisica Sperimentale – OGS Trieste, Italy, a mesocosmos experiment was performed in order to decode how different sources (natural, anthropogenic) of CO<sub>2</sub> influence biological systems (phytoplankton) using stable carbon isotopes. The results are in progress.

Stable isotopes of C and N were also used in the research of **palaeoclimatic changes** at the Ljubljana Marshes. Research is conducted in collaboration with ZRC-SAZU. Our results were compared with results from other sites in different regions of Slovenia and Europe, to better understand the intensity, timing and spatial framework of environmental processes over the last 15,000 years and the emergence of today's cultural landscape.

### Microbial ecology

The microbial system ecology is focused on the interaction of microbes with surfaces, particularly the colonisation and tripartite bio-physico-chemical processes occurring on surfaces. The human biomonitoring is focused on elucidation of the biological and chemical processes that put in the increasing risk of particular human subpopulations. In both research activities we use molecular biology, chemical analytics and nanotechnology-based methods.

Under the microbial system ecology activities, in 2016 we successfully started a national basic research project involving partners from Medical Faculty (MFUM) Faculty of Mechanical Engineering (FMEUM), both from the University of Maribor, in addition to Faculty of Pharmacy (FP) from the University of Ljubljana aiming to determine the electrostatic interaction of bacteria with surfaces as well as their biological responses. Supporting this research through the establishment of a cooperation with the Saratov State University (SSU) from Russian Federation and Queen Mary University of London, UK, via a governmentally supported bilateral project, enabled us to elucidate the effects of polyelectrolytes on the bacterial division at the single-cell level.

The **electrostatic attachment of alive bacterial cells**, developed under the ongoing project, has been applied within a few national projects: in cooperation with MFUM and FMEUM we developed special patches that incorporate beneficial bacteria and in cooperation with FP and University Clinical Centre from Ljubljana we have been developing the active polymeric sol-gel structure incorporating beneficial bacteria preventing either ulcers on diabetic feet or the development of periodontal disease, respectively. Using electrostatic attachment and in cooperation with researchers from Belgium, Netherlands and Denmark we also developed the strategy to clean 2,6-dichlorobenzamide (BAM)



Figure 1: Sampling at the Sava River; Serbia, September 2016.

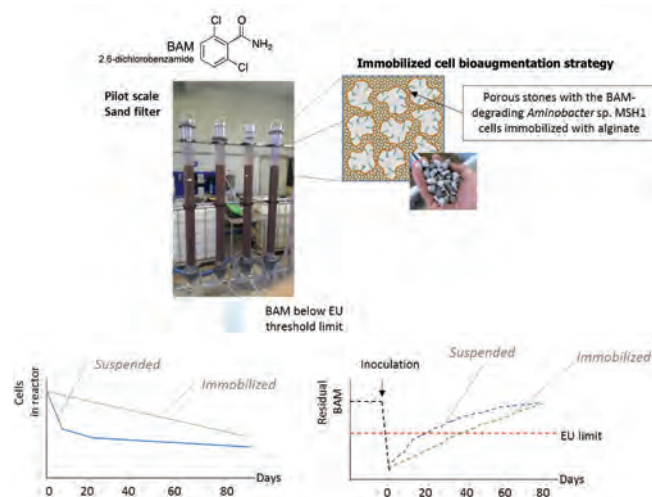


Figure 2: Applicative solution for the use of immobilized bacterial cells for the degradation of xenobiotics, as presented for the case study of a pesticide residual BAM.

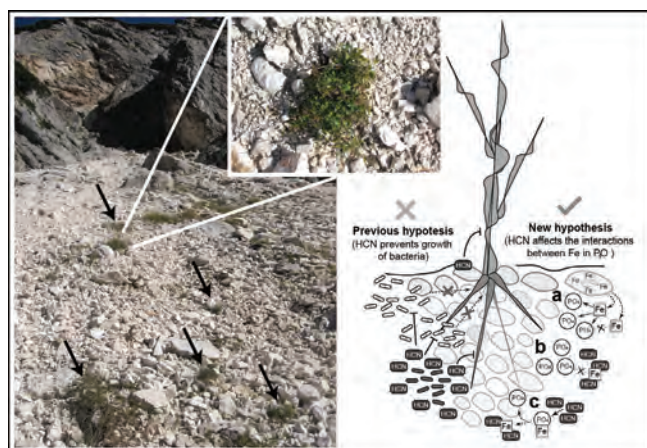


Figure 3: In oligotrophic environments, where the nutrients are stored in the raw bedrock, bacteria producing HCN interfere with processes of co-precipitation of iron with phosphate, which indirectly increase the availability of phosphorous.

polluted drinking water by applying BAM degrading bacteria (Fig. 2). Using this approach we were able to increase the durability of the filter and decrease the operating costs. The manuscript based on the insights of this approach has been accepted in the Environmental Science and Technology journal. This year, on the same principle of electrostatic attachment of bacteria, we also applied the first stage of the H2020 call under topic “Architected/Advanced Material Concepts for Intelligent Bulk Material Structures” to develop a self-healing concrete mixture.

In 2016 we achieved a major breakthrough in the research of the physiology of attached microbes on plants roots. We were able to determine the involvement of HCN producing bacteria in the processes of the P uptake by plants. Based on our analysis we disregarded the decades-long hypothesis that HCN producing bacteria present in this ecosystem act against plant pathogenic bacteria, but we gave alternative one where HCN produced by bacteria sequester Fe by formation of complexes. In return, plants can obtain more P due to its increased bioavailability. We published these insights in the prominent journal *Frontiers in Microbiology* (Fig. 3).

### Environment and health

The human biomonitoring activities LIFE+ project CROME (Cross-Mediterranean Environment and Health Network), coordinated by the University in Thessaloniki (AUTH), finished at the end of December 2016. In this project, an advanced methodology was applied for identifying associations between environmental stressors (mainly pollutants from the environment), metabolism, genetic background, and subclinical or clinical health effects. Re-sampling of birth cohort established within the PHIME project was successfully finished with the collaboration of the Children’s Hospital in Ljubljana. Children, now 7-8 years old, were re-assessed for internal exposure to metal(loid)s and cognitive performance by psychologists using standard intelligence tests. Data analysis performed so far, indicated the importance of a genetic component in the response to environmental stress, particularly, negative association between mercury prenatal exposure and cognitive function at 18 months of age was observed, which was dependent on the apolipoprotein E gene polymorphism.

Based on the existing data from the national HBM, we showed the importance of using appropriate biomarkers of exposure in such studies, particularly for cadmium. We also critically evaluated biomarkers of kidney damage, which are also assessed at low levels of exposure, the levels that

are typical for general, not occupationally exposed populations. In addition to this, we investigated associations between concentrations of metals in samples, either essential or potentially toxic, and birth weight, taking into account potential life-style and numerous other factors that could influence birth weight.

Following similar aims and using the same methods, in the frame of the FP7 project HEALS we have harmonized and prepared a protocol for a study that is including the recruitment of twins and singletons, to investigate a role of genetic, epigenetic, metabolic and other factors in response to environmental stress in the most vulnerable period of life. Recruitment of this new study population is foreseen to be conducted at the beginning of 2017.

In the framework of the Minamata convention we have conducted a methodological workshop (*Monitoring exposure to and environmental concentrations of mercury*) under the World Health Organization (WHO), which was intended for national coordinators and laboratory analysts from participating countries.

We were also actively involved in the preparation of a proposal for European HBM (HBM4EU), starting on the 1st of January 2017, in which we are taking the leading part in the workpackage focused on cadmium and chromium.

At the beginning of October we started with activities in the frame of CRP project (*Exposure of children and teenagers to selected chemicals in the living environment*), which is also coordinated by our department. We prepared a criteria-based review of chemicals, based on which the most relevant will be selected for monitoring in specific population groups.

In a dwelling with elevated air radon concentration (in winter up to 16 kBq m<sup>-3</sup>), situated in the Slovene Karst, the temporal and spatial distribution of radon has been studied and its main source sought. Extremely high radon levels in summer (during a weeklong absence of residents it reached 20 kBq m<sup>-3</sup>), led us to the conclude

that the strong radon source is not the basement with earthen floor, but rather a hidden karst cave near or even under the house in the part without the basement. Due to the prevailing karst in our country, more such cases could be expected.

Determinations of the number concentration of **nanoparticles** (10–1100 nm) and their size distribution have been performed (within a bilateral cooperation with Serbia) in wintertime in several dwellings, whose heating is based on burning wood in a stove. *This process* emitted particles mostly smaller than 100 nm, with an average particle generation rate from  $1.1 \times 10^{10}$  to  $1.5 \times 10^{11} \text{ min}^{-1}$ . Similarly, smoking a cigarette released up to  $2.4 \times 10^{11}$  particles  $\text{min}^{-1}$ , only they were larger, i.e., 200 nm.

In biomedical research, in collaboration with other departments from JSI, pH and **metal concentration of synovial fluid of osteoarthritic joints** and joints with metal replacements have also been studied.

In cooperation with Oncology Institute from Ljubljana, magnetic field was applied, enhancing the cellular uptake for effective therapy with magnetofection, using plasmid DNA encoding against Mcam in B16F10 melanoma in vivo. Cytotoxic trans-platinum(II) complex with 3-hydroxymethylpyridine was synthesised and its structure characterised by x-ray spectrometry. The complex was evaluated regarding its biological activity. The study was also performed on electrochemotherapy by pulsed electromagnetic field treatment in mouse melanoma B16F10 in vivo.

In a collaboration with University Medical Centre Ljubljana we continued with a study of **arsenic metabolism in acute promyelocytic leukaemia** patients treated with arsenic trioxide. Our results suggest the possibility of unpredictable exceptions in the metabolism of individual patients, which are important in terms of individual dose adjustment. We assume that the causes lie mainly in the interaction of additional disease states and/or additional drugs and to a lesser extent in genetics. We also followed metabolites of arsenic and polymorphisms of selected genes (*ASMT*, *SELP*, etc.) in the general population with a nutritional intake of arsenic - pregnant women, sea food.

In the arsenic speciation field, we also studied the metabolism of **arsenic in plants** and were involved in the development of new methods for the determination of the total arsenic in solid samples using laser ablation and atomic fluorescence spectrometry.

**Cr(III)-EDTA, Cr(VI) and Cr(III)-nitrate cytotoxic and genotoxic activity** was studied in the human **hepatoma** (HepG2) cell line and the influence of non-cytotoxic concentrations of contaminants on DNA damage was determined with the comet assay. Cell viability was decreased only by Cr(VI) at concentrations above  $1.0 \text{ mg mL}^{-1}$ . Cr(VI) at  $0.2 \text{ mg mL}^{-1}$  and Cr(III) at  $1.0 \text{ mg mL}^{-1}$  induced DNA damage, while Cr(III)-EDTA exposure did not form DNA strand breaks.

#### Food research and activities of the ERACHair ISO-FOOD

The ISO-FOOD - ERA Chair for isotope techniques in food safety, quality and traceability was established in 2014. Work is ongoing on the studies of potential robust indicators for determining the geographical origin and discriminating amongst various types of production regimes for vegetables (lettuce, sweet pepper, tomato, potato, garlic). Stable isotopes of carbon, nitrogen, oxygen and sulphur, as well as elemental composition (P, S, Cl, K, Ca, Si, Ti, Zn, Br, Rb and Sr) were analysed in order to determine the geographical origin of vegetables at the scale of Slovenia and also Southern and Central Europe and the Mediterranean. Additionally, rare-earth elements (La, Pr, Nd, Dy), other macro and micro elements (Na, Mg, Cr, Mn, Fe, Co, Ni, Cu, Zn, Mo, Cd, Cs, Pb) and chemical-physical parameters (antioxidant potential, total phenolics, vitamin C, carotenoids, ammonium, nitrites and nitrates) were also used in some cases. The preliminary results show good potential for the discrimination according to the geographical origin. The influence of different fertilizing regimes on nitrogen isotopic fingerprints in vegetables in combination with morphological characteristics was evaluated in pot experiments with garlic, sweet pepper and carrots. Results show differences among different types of production regimes.

Furthermore, we investigated the possibility of determining the **geographical origin of milk** and milk products. Our study contains a combination of multi-elemental composition and the analysis of stable isotopes of light elements for genuine samples of milk and cheeses from different geographical areas of Slovenia. Using linear discriminant analysis discrimination and specification of goat, cow and sheep milk and cheese was possible. Based

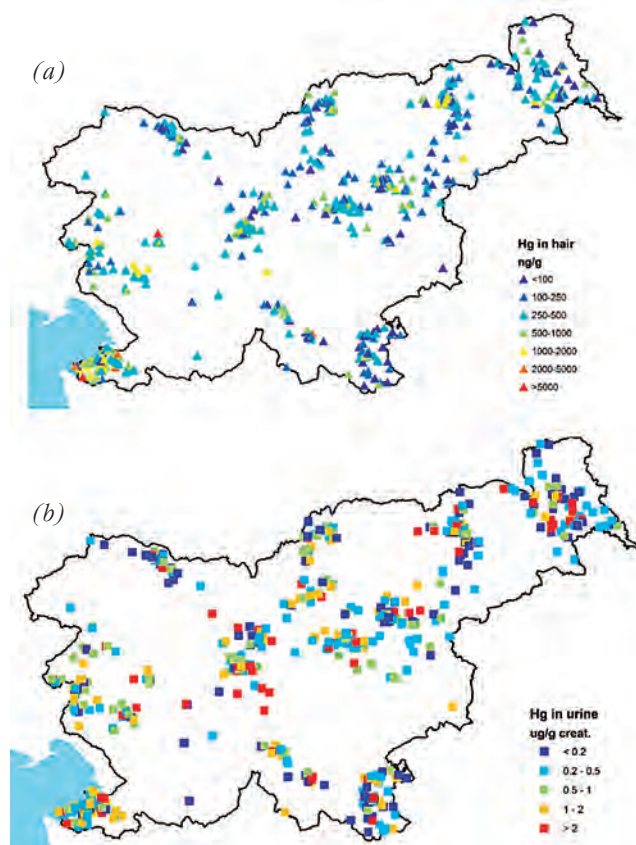


Figure 4. Distribution of Hg in Slovenian population (a) hair values reflect Hg uptake from frequent consumption of fish (b) urine Hg values reflect Hg uptake from amalgams.

on a database of genuine Slovenian milk, which was supplemented from 2012, we have developed a statistical model based on which it is possible to verify whether the milk is really produced in Slovenia. The model was tested on 30 samples of milk available on the Slovenian market arising from different European countries. Slovenian milk was statistically distinguishable from all other milk, where the most important parameters were:  $\delta^{18}\text{O}$ , Sr, K and Ca.

Furthermore, our research performed in the **smart-specialization program "Food for Future"** started with method optimization for active components detection with GC-MS-SPME and preliminary testing of selected analytical systems and methods. Commercially available distillate of apples were analysed to obtain the best analytical conditions that could be further used for stable isotope analysis. This research is performed in collaboration with Frutarom Etol company.

In cooperation with the Institute for Hop Research and Brewing, we examined the usefulness of stable isotopes of light elements (C, H, N and S) in the **differentiation of hops from different geographical areas**. The first studies have not given encouraging results, so we decided to expand our research into the determination of the isotopic composition of H and O in hops.

In laboratory-based conditions, the **soil-to-plant transfer of uranium, thorium, radium and lead** for radish, savoy and rocket was investigated on soils contaminated with uranium-mill tailings. Different levels of soil contamination under various growing conditions were applied in a pot experiment to simulate different contamination scenarios. The results obtained indicate a significant linear correlation between the content of the radionuclides in the soil and plants as well as between content of the radionuclides in plants and pedological parameters, while contamination has no effect on the photochemical efficiency and the content of photosynthetic pigments in the selected plants.

In the research field of nanoparticles, we cooperated with the Department of Nanostructured Materials and the Department of Physics of Complex Matter. We have investigated the **properties of nanoparticles** that can be found in the food, the interactions between the organic substance and the nanoparticles activated by light, and the potential for transfer of substances contained in nanoparticles in food and their transfer to human tissues.

Also, this year ISO-FOOD organized Exploratory Workshop entitled "Isotopic techniques in food characterization" with seven invited speakers from different topics, including metrology and preparation of reference materials, the use of different instruments for stable isotope analysis, statistical evaluation and modelling and formation of "isoscapes" in food traceability. In total, the workshop attracted 46 participants from nine different countries.

### Environmental technologies

We performed a series of **photo and bio-degradations of sertraline**, where photodegradation experiments with pH-related experiments were carried out and an experiment where sensitizers such as riboflavin, rose bengal and anthraquinone-2-sulfonic acid were applied. In the case of bisphenol alternatives, we have begun the incubation of suspended and attached growth biomass reactors with a mixture of 18 BPA alternatives.

A work was performed on the chemical characterisation of dredged sediments from Luka Koper. The data indicated that due to the large amounts of sediment available, civil engineering applications such as the construction of embankments is the most beneficial recycling solution at present.

The **leaching protocols** available for the evaluation of the long-term environmental impacts of building composites containing waste materials were critically assessed. New leaching tests based on the diffusion and dissolution of contaminants were proposed using synthetic surface and seawater as the leaching solutions.

For an accurate determination of **TiO<sub>2</sub> nanoparticles (NPs)**, sample treatments, which maintain NPs dispersed and stabilized in solution, enabling quantitative transfer of TiO<sub>2</sub> NPs during the analytical procedure, are of crucial importance. Dispersion approaches using different mechanical and ultrasonication procedures in combination with various dispersing agents were examined. Results demonstrated that different environmental conditions (natural organic matter, ionic strength) have a significant influence on the efficiency of dispersion and the stability of TiO<sub>2</sub> NPs, revealing that for each environmental matrix, different dispersion approach needs to be applied.

**Iron nanoparticles (FeNPs)** are frequently applied in the remediation of contaminated environmental waters. If FeNPs remain in these waters after the treatment, they can cause hazardous effects to the environment. A time-dependent size distribution of FeNPs was investigated in Milli-Q water, forest spring water and landfill leachate after the different FeNPs treatments. The data revealed that settling and removal of FeNPs after the treatment of waters was related to the sample characteristics and the ways of NPs dispersion. When mixing was used for the dispersion the FeNPs quickly settled. Dispersion with TMAH resulted in a slower settling of iron aggregates, and thus may represent a potential threat in environmental waters with low ionic strength.

In collaboration with other departments from the JSI, dissolution mechanism of upconverting AYF<sub>4</sub>:Yb,Tm (A = Na or K) nanoparticles in aqueous media was investigated.

### Environmental management, environmental impact assessment and risk assessment

In September the CITI-SENSE project ended, an EU project aimed to test and develop air-quality related *Citizens' observatories* (CO) in nine cities across the Europe, Ljubljana being one of pilot cities. The general public, schools and other interested were involved in the project through hosting some of the AQ sensor devices, as well as providing feedback on developed tools and applications. As part of awareness raising campaigns on air quality issues and novel sensor technologies, workshops, information days, activities in the nature as well as in the city centre were organised throughout the lifetime of the project.

In 2016 the work on a 4 year H2020 ICARUS project started (ICARUS stands for Integrated Climate forcing and Air Pollution Reduction in Urban Systems).

We commenced a 2-year national research project "Potential substances of very high concern in the context of REACH regulation" in the framework of the Targeted research programme 2016.

Additionally, second phase of the site suitability evaluation for the new LPG storage facility at Steklarna Hrastnik d.o.o. has been made, and an opinion for the NPP Krško regarding obligations associated with Environmental Impact Assessment procedure for its lifetime extension by 2043 has been provided.

### Environmental monitoring

In collaboration with the Environmental Agency from Croatia monitoring of organotin compounds and polybrominated diphenyl ethers in surface and sea water started in 2016. The monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski vrh was performed. We also participated in off-site monitoring of Krško Nuclear Power Plant (NPP) with a determination of strontium and tritium in environmental samples. The monitoring of tritium and radiocarbon in gas effluents from the NPP was also performed. With analyses of strontium and tritium we also participated in the monitoring of radioactivity in drinking water in Slovenia, as well as in the monitoring of the living environment in Slovenia. Methods used for the determination of strontium, tritium and radiocarbon for the monitoring purposes are accredited by the Slovenian accreditation body (SA LP-090).

### Infrastructural Centre for Mass Spectrometry (CMC)

The mass spectrometric measurements are involved in many research programs and projects in the field of environmental chemistry, chemistry for sustainable development, synthesis and medicinal chemistry, biochemistry, medicine and other natural sciences with research groups at JSI, the National institute of Chemistry, National institute of Biology, University of Ljubljana, Maribor and Nova Gorica, Centers of excellence: One-fist, CIPKeBiP, Namaste et al.

With a high-resolution tandem mass spectrometer QToF Premier, LC-MS and GC-MS analyses were identified and determined the structure of many organic compounds, organic-metallic complexes, biopolymers and similar compounds. We studied the new synthesized organic compounds, the bioactive substances, proteins, lipids and similar organic molecules, ceramic materials, food supplements and food additives, monitoring pollutants in the environment, etc.

An example of such research, in collaboration with the Faculty of Pharmacy at University of Ljubljana and the National institute of Chemistry, was a publication in the prestigious scientific journal *Angewandte Chemie*, where we explained the function of a new type of potential target drugs to selective inhibition on immunoproteasome. This would improve the treatment of autoimmune disease and cancer. The coupling of liquid chromatography and mass spectrometry were also used for the characterization of organic acids in the complex compounds of nickel in plants for the bioremediation of the degraded environment, chemical analysis of a mixture of fatty acid derivatives, lipids, cholesterol in biological membranes, cytostatic bleomycin in the blood serum and tumour tissue, quantitative determination of cannabinoids in preparations of medical hemp and many other MS applications.

The Department of Environmental Sciences also operates a mobile chemical laboratory ELMU (Ecological Laboratory with a Mobile Unit) which is organized in the system of Slovenian Civil Protection as a unit for the intervention in ecological accidents with hazardous substances and materials. The chemical mobile unit had four interventions in 2016, mainly due to chemical accidents and environmental pollution of toxic compounds. A new vehicle mobile chemical laboratory ELMU is on standby to provide ecological accidents with hazardous substances, and also serves for the sampling of water, air and soil from the environment.

### Some outstanding achievements

1. A study of the fate of iron nanoparticles (FeNPs) in contaminated environmental waters treated with nanoscale zero-valent iron, FeONPs and Fe<sub>3</sub>O<sub>4</sub>NPs. The investigation significantly contributed to understanding the mechanisms and kinetics of FeNPs settling and their removal from remediated waters, which is essential to prevent nano-threat to living organisms.



2. Mathematical model for determination of origin of precipitation based on linear combination of  $\delta^3\text{H}$  and  $\delta^{18}\text{O}$  values and quantity of precipitation connected to air circulation, developed in 2015, was selected as excellent achievement in hydrogeology field by the ARRS in 2016.
3. Involvement in the new smart specialization program: Food for Future and active participation in SRIP – Food.
4. Based on our analysis we disregarded the decades-long hypothesis that HCN producing bacteria present in this ecosystem act against plant pathogenic bacteria, but we gave alternative one where HCN produced by bacteria sequester Fe by the formation of complexes. In return, plants can obtain more P due to its increased bioavailability.
5. We developed the strategy to clean 2,6-dichlorobenzamide (BAM) polluted drinking water applying electrostatically attached BAM degrading bacteria. Using this approach we were able to increase the durability of the filter and decrease the operating costs.
6. We have demonstrated the importance of apolipoprotein E genetic variability in association between low-level mercury exposure, typical for the Slovenian population, and the cognitive performance of children.
7. Contribution to the extended operation of Nuclear Power Plant Krško until 2043.
8. In the framework of the MAASTWIN project capacity building in novel mass spectrometry techniques have commenced.

### Some outstanding publications in the past year

1. K. Peeters, G. Lespes, T. Zuliani, J. Ščančar, R. Milačič. The fate of iron nanoparticles in environmental waters treated with nanoscale zero-valent iron, FeONPs and Fe<sub>3</sub>O<sub>4</sub>NPs. *Water Research*, 2016, 94, 315-327.
2. P. Novak, T. Zuliani, R. Milačič, J. Ščančar. Development of an analytical method for the determination of polybrominated diphenyl ethers in sewage sludge by the use of gas chromatography coupled to inductively coupled plasma mass spectrometry. *Analytica Chimica Acta*, 2016, 915, 27-35.
3. T. Kosjek, A. Krajnc, T. Gornik, D. Žigon, A. Grošelj, G. Serša, M. Čemažar. Identification and quantification of bleomycin in serum and tumor tissue by liquid chromatography coupled to high resolution mass spectrometry. *Talanta*, 2016, 160, 164-171.
4. M. Zdanowicz, E.M. Krümmel, A.J. Poulain, E. Yumivhoze, J. Chen, M. Štok, M. Scheer, H. Hintelmann. Historical variations of mercury stable isotope ratios in Arctic glacier firn and ice cores. *Global biogeochemical cycles*, 2016, 30, 1324-1347.
5. A. Bratkič, M. Vahčić, J. Kotnik, K. Obu, E. Begu, M.E. Woodward, M. Horvat. Mercury presence and speciation in the South Atlantic Ocean along the 40°S transect. *Global biogeochemical cycles*, ISSN 1944-9224, 2016, 30, 105-119.
6. A. B. Kopal, J. Snoj, D. Tratnik, D. Maze, V. Fajon, D. Gibičar, A. Miklavčič, d. Kocman, J. Kotnik, A. Briški, J. Osredkar, M. Krsnik, M. prezelj, Č. Knap, B. Križaj, L. Liang, M. Horvat. Exposure to mercury in susceptible population groups living in the former mercury mining town of Idrija, Slovenia, *Environmental Research*, 2016, in press.
7. K. Bat, K. Eler, D. Mazej, B. Mozetič Vodopivec, I. Mulič, P. Kump, N. Ogrinc. Isotopic and elemental characterisation of Slovenian apple juice according to geographical origin: preliminary results. *Food chemistry*, 2016, 203, 86-94
8. B. Horemans, B. Raes, J. Vandermaesen, Y. Simanjuntak, H. Brocatus, J. T'Syen, J. Degryse, J. Boonen, J. Wittebol, A. Lapanje, S.R. Sørensen. D. Springael. Biocarriers improve bioaugmentation efficiency of a rapid sand filter for the treatment of 2, 6-dichlorobenzamide (BAM)-contaminated drinking water. *Environmental science & technology*, in press 2016, 28p.
9. T. Rijavec, A. Lapanje. Hydrogen cyanide in the rhizosphere: not suppressing plant pathogens, but rather regulating availability of phosphate. *Frontiers in microbiology*, in press 2016, 45p.
10. B. Kontić, M. Bohanec, D. Kontić, N. Trdin, M. Matko. Improving appraisal of sustainability of energy options - a view from Slovenia, *Energy Policy*, 2016, 90, 154-171.

### Organization of conferences, congresses and meetings

1. Milena Horvat: WHO Training workshop for national coordinators and laboratory analysts in the frame of the UNEP/WHO project "Development of a Plan for Global, Monitoring of Human Exposure to and Environmental Concentrations of Mercury", Reaktorski center Podgorica, Ljubljana, Slovenia, 8–12 February 2016
2. MAASTWIN Kick-off meeting; Reactor Centre Podgorica, Ljubljana, Slovenia, 29–30 March 2016
3. Iso-Food Workshop on speciation of trace elements: Mercury speciation in food and the global mercury cycle; Reactor Centre Podgorica, Ljubljana, Slovenia, 46 April 2016

4. ISO-FOOD Summer School: Radionuclides in food; Reactor Centre Podgorica, Ljubljana, Slovenia, 6–10 June 2016
5. GLOBAQUA training course “The use of stable isotopes in investigations of hydrological processes and climate change”, Reactor Centre Podgorica Podgorica, Ljubljana, 10–13 October 2016
6. CROME-LIFE Inter-regional Workshop, Reactor Centre Podgorica, Ljubljana, Slovenia, 24–25 November 2016
7. MASSTWIN Group training “Metrology in measurements of stable isotopes of light elements: traceability, uncertainty and comparability”, Reactor Centre Podgorica, Ljubljana, Slovenia, 7 December 2016
8. ERA-Chair ISO-FOOD Exploratory Workshop »Isotopic Techniques in food characterisation«, Reactor Centre Podgorica, Ljubljana, Slovenia, 8–9 December 2016
9. 14RPT-03-ENVCRM Project Midterm Meeting, “EMPIR; ENVCRM—Matrix reference materials for environmental analysis”, Reactor Centre Podgorica, Ljubljana, Slovenia, 13–14 December 2016

## Patent granted

1. Aleš Lapanje, The impregnation process and attachment of microorganisms in porous materials, SI24910 (A), Slovenian Intellectual Property Office, 29. 07. 2016.

## INTERNATIONAL PROJECTS

- |  |  |
|--|--|
| <ol style="list-style-type: none"> <li>1. Analyses of Metals, TBT and DBT in Sediments, Mussels and Fish<br/>Prof. Janez Ščančar<br/>Analyses of the Swiss Moss Samples in the Framework of the UNECE ICP Vegetation Programme<br/>Asst. Prof. Zvonka Jeran<br/>Fub Ag</li> <li>2. 7FP - CITI-SENSE; Development of Sensor-based Citizens' Observatory Community for Improving Quality of Life in Cities<br/>Prof. Milena Horvat<br/>European Commission</li> <li>3. 7FP - HEALS; Health and Environment-wide Associations Based on Large Population Surveys<br/>Prof. Milena Horvat<br/>European Commission</li> <li>4. 7FP - GLOBAQUA; Managing the Effects of Multiple Stressors on Aquatic Ecosystems Under Water Scarcity<br/>Prof. Radmila Milačič<br/>European Commission</li> <li>5. 7 FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability<br/>Prof. Milena Horvat<br/>European Commission</li> <li>6. LIFE12 ENV/ - CROME-LIFE; Cross-Mediterranean Environment and Health Network<br/>Prof. Milena Horvat<br/>European Commission</li> <li>7. MeTra; EMRP - Traceability for Mercury Measurements<br/>Prof. Milena Horvat<br/>Euramet E.v.</li> <li>8. EMPIR; ENVCRM - Matrix Reference Materials for Environmental Analysis<br/>Prof. Milena Horvat<br/>Euramet E.v.</li> <li>9. STAWA; Towards the Assessment of Ecological Status of Water Bodies in the Sava River Basin<br/>Prof. Radmila Milačič<br/>Eurovienna - Eu-consulting &amp; -management Gmbh</li> <li>10. COST ES1403 - New and Emerging Challenges and Opportunities in Wastewater Reuse (NEREUS)<br/>Prof. Ester Heath<br/>Cost Office</li> <li>11. LIFE RusaLCA-Nanoremediation of water from small waste water treatment plants and reuse of water and solid remains for local needs<br/>Prof. Janez Ščančar<br/>European Commission</li> <li>12. 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...<br/>Prof. Nives Ogrinc<br/>IAEA - International Atomic Energy Agency</li> <li>13. Stability Monitoring of ERM-EF411, ERM-EF412 &amp; ERM-EF413<br/>Dr. Radojko Jačimović<br/>Institute For Reference Materials And Measurements</li> <li>14. Training Fees for Ms Delali Tulasi, (Ghana), 01.01. - 31.07.2016</li> </ol> | <ol style="list-style-type: none"> <li>Prof. Milena Horvat<br/>International Centre for Theoretical Physics</li> <li>15. Stability Monitoring of the Certified Reference Material ERM-CZ120<br/>Asst. Prof. Tea Zuliani<br/>Institute For Reference Materials And Measurements</li> <li>16. Stability Monitoring of ERM-EC590 and ERM-EC591<br/>Dr. Radojko Jačimović<br/>Institute For Reference Materials And Measurements</li> <li>17. Develop Training Modules as a Component of a Training Course Mercury and Implementation of the Minamata Convention in the Health Sector<br/>Prof. Milena Horvat<br/>World Health Organization</li> <li>18. BCR-679 White Cabbage and ERM-CD281 Rye Grass<br/>Prof. Milena Horvat<br/>Institute For Reference Materials And Measurements</li> <li>19. Stability Monitoring of Certified Reference Material BCR-185R (Bovine Liver)<br/>Asst. Prof. Tea Zuliani<br/>Institute For Reference Materials And Measurements</li> <li>20. Development of a Plan for Global Monitoring of Human Exposure to and Environmental Concentrations of Mercury<br/>Prof. Milena Horvat<br/>World Health Organization</li> <li>21. Training Fees for Mr Dalerjon Khojiboev (Tajikistan), 25.4.2016 - 27.7.2016<br/>Prof. Ljudmila Benedik<br/>International Centre for Theoretical Physics</li> <li>22. Stability Monitoring of ERM-EC680m and ERM-EC681m<br/>Dr. Radojko Jačimović<br/>European Commission</li> <li>23. Training Fees for Mr Kyrlyo Korychenskyi (Ukraine), 10.9.2016 - 9.12.2016<br/>Prof. Borut Smodiš<br/>International Centre for Theoretical Physics</li> <li>24. Training Fees for Mrs Delali Tulasi (Ghana), 17.9.2016 - 16.1.2017<br/>Prof. Milena Horvat<br/>International Centre for Theoretical Physics</li> <li>25. IAEA Fellowship for Mr Faisal J H H A Alabasey (KUW/16016), 17.10.2016-16.11.2016, IAEA Project: Upgrading National Nuclear Analytical Capabilities for Environmental and Foodstuff Radioactivity<br/>Prof. Janja Vaupotič<br/>IAEA - International Atomic Energy Agency</li> <li>26. H2020 - ERA-PLANET; The European Network for Observing Our Changing Planet<br/>Prof. Milena Horvat<br/>European Commission</li> <li>27. H2020 - ICARUS; Integrated Climate Forcing and Air Pollution Reduction in Urban Systems<br/>Prof. Milena Horvat<br/>European Commission</li> <li>28. H2020 - MASSTWIN; Spreading Excellence and Widening Participation in Support of Mass Spectrometry and Related Techniques in Health, Environment, and Food Analysis<br/>Prof. Milena Horvat<br/>European Commission</li> <li>29. Exposure-response Assessment of Ambient Air Pollution (AAP) and Hg Contamination in Affected Cities of India and Slovenia: A Comparative Study</li> </ol> |
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- Prof. Milena Horvat  
Slovenian Research Agency
30. The Use of New Methods for Dating Young Groundwater in Slovenia  
Prof. Nives Ogrinc  
Slovenian Research Agency
  31. Screening of Organic Pollutants and their Effects in Water  
Prof. Ester Heath  
Slovenian Research Agency
  32. Anthropogenic Radionuclides in the Sava River and their Transboundary Effects  
Dr. Marko Štok  
Slovenian Research Agency
  33. Air Pollution Monitoring, Maps and Tools for Assessment of Exposure to Selected Pollutants in Slovenia and Serbia  
Dr. David Kocman  
Slovenian Research Agency
  34. Trace Metals Partitioning between Water Column, Suspended Particulate Matter and Sediments of the Sava River  
Prof. Janez Ščančar  
Slovenian Research Agency
  35. Assessment of Emerging Contaminants in the Sava River  
Prof. Ester Heath  
Slovenian Research Agency
  36. Effects of Electrostatic Modifications of Bacterial Cells on their Physiology: Growth, Division, Expression  
Dr. Aleš Lapanje  
Slovenian Research Agency
  37. Promotion of Slovenian Science and Slovenia in the Framework of "Division of Chemistry and Environment" within "European Association for Chemical and Molecular Sciences"  
Prof. Milena Horvat  
Slovenian Research Agency

## RESEARCH PROGRAMS

1. Modelling and environmental impact assessment of processes and energy technologies  
Prof. Borut Smodiš
2. Cycling of substances in the environment, mass balances, modelling of environmental processes and risk assessment  
Prof. Milena Horvat

## R&D GRANTS AND CONTRACTS

1. Development of Molecularly Imprinted Polymers and their application in environmental and bio-analysis  
Asst. Prof. Tina Kosjek
2. Vegetation and hydrology of Ljubljansko barje in the past, present and future a consequence of succession, human impact or climatic fluctuations?  
Prof. Nives Ogrinc
3. Modelling hydrologic response of nonhomogeneous catchments  
Prof. Sonja Lojen
4. Electrostatic immobilisation of bacterial cells and effects on their physiology  
Prof. Milena Horvat
5. The effect of iodine and selenium on growth and quality of crops  
Prof. Vekoslava Stibilj
6. Bisphenol A alternatives: transfer from food contact material, fate and human exposure  
Prof. Ester Heath
7. Spatial distribution of water isotopes in precipitation in Europe with special fokus on the transect from the Adriatic Coast to the Pannonian Plain  
Dr. Polona Vreča
8. Comparative study of ecosystem management and services in contrasting Slovenian freshwater systems  
Dr. David Kocman
9. In-situ remediacija onesnažene zemljine na področju stare Cinkarne In-situ remediation of polluted grounds in the area of the Zink-works at Celje  
Prof. Janez Ščančar
10. Improved treatment and monitoring of Water Framework Directive priority pollutants  
Prof. Ester Heath
11. Optimization and validation of new indicator systems in complex environmental

- matrices  
Prof. Milena Horvat
12. Evaluating geological sequestration of CO<sub>2</sub> in low rank coals; Velenje basin, Slovenia as a natural analogue  
Dr. Tjaša Kanduč
  13. Pharmaceutical and personal care product residues in the environment: Occurrence, sources, treatment and effects  
Prof. Ester Heath
  14. 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
  15. 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
  16. Exposure of children and adolescents to selected chemicals through their habitat environment  
Prof. Milena Horvat
  17. Potential substances of very high concern in the context of REACH regulation  
Dr. Davor Kontić
  18. In situ immobilization of contaminated soil using innovative nanotechnology, for processing and use as urban soils  
Prof. Radmila Milačič
  19. In situ immobilization of contaminated soil using innovative nanotechnology, for processing and use as urban soils  
Prof. Radmila Milačič
  20. Slovenian National Implementation Plan for the Minamata Convention on Mercury  
Dr. David Kocman
  21. EMRP; MeTRA - Traceability for Mercury Measurements  
Prof. Milena Horvat
  22. Services; Determination of the Isotopic Composition of Carbon in Sugar Samples  
Prof. Nives Ogrinc
  23. Different Analyses  
Prof. Sonja Lojen
  24. Provision of Testing Services for Filter Media used in IMS Radionuclide Stations  
Prof. Ljudmila Benedik  
The Preparatory Commission For The Comprehensive
  25. Small Services in the Years from 2007 to 2016  
Prof. Milena Horvat
  26. Determining Elemental Content in Environmental Samples Using k<sub>0</sub>-INAA  
Dr. Radojko Jačimović
  27. Irradiation and Analysis of Nano SiC Samples  
Dr. Radojko Jačimović  
National Nuclear Research Center
  28. The Use of Stable Isotopes in Investigations of Hydrological Processes and Climate Change  
Prof. Nives Ogrinc
  29. Food for future - F4F  
Prof. Nives Ogrinc

## NEW CONTRACTS

1. 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
2. Analyses of atmospheric releases in 2015, 2016 and 2017  
Dr. Marko Štok  
Krško Nuclear Power Plant (NEK)
3. Environmental radioactivity monitoring of living environment in Slovenia in 2015  
Dr. Marko Štok  
Ministry of the Environment and Spatial Planning
4. Off-site radiological monitoring of the Krško Nuclear Power Plant in 2016 and 2017  
Dr. Marko Štok  
Krško Nuclear Power Plant (NEK)
5. Environmental radioactivity monitoring of living environment in Republic Slovenia in 2016  
Dr. Marko Štok  
Ministry of the Environment and Spatial Planning
6. Monitoring of radioactivity in drinking water in Republic of Slovenia in 2016 and 2017  
Dr. Marko Štok  
Ministry of Health of the Republic of Slovenia

## VISITORS FROM ABROAD

1. Dr Sergio Ribeiro Guevara, Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Bariloche, Argentina, 17 January to 6 February 2016
2. Jarmila Makovinska, Emilia Elexova Miškova, Water research Institute, Bratislava, Slovakia, 9–12 February 2016
3. Stefan Andus, Marija Ilić, Nikola Marinković, Durad Milošević, Miroslava Mitrović, Boris Novaković, Miroslav Očadilnik, Momir Paunivici, Marina Piria, Nataša Popović, Predrag Simonović, Jelena Đuknić, Jelena Vičanović, University of Belgrade, Institute for Biological Research "Sinisa Stankovic", Belgrade, Serbia, 9–12 February 2016

4. Dr Dominika Saniewska, Department of Marine Chemistry and Environmental Protection, Institute of Oceanography, University of Gdańsk, Gdańsk, Poland, 29 February to 25 March 2016
5. Diana Babi, Tekran® Instruments Corporation, Totonto, Canada, 10–14 March 2016
6. Dr Bourquin Maurice Henri Césa Eric, Elżbieta Marta Nowak, CERN, Geneva, Switzerland, 21–23 March 2016
7. Prof. Akagi Hirokatsu, International Mercury Laboratory Inc., Minamata, Kumamoto, Japan, 15 April to 12 May 2016
8. Dr Arne Jernelöv, ex-director International Institute of Applied Systems Analysis in Vienna, Vienna, Austria, 28 April to 1 May 2016
9. Dalerjon Khojiboev, Department of Ecology, Faculty of Metallurgy, Mining-Metallurgical Institute of Tajikistan, Sogd region, Chkhalovsk, Tadjikistan, 25 April to 30 July 2016
10. Theo Bulteau, Université François Rabelais – Département Géosciences-Environnement – Faculté des Sciences et Techniques, Tours, France, 27 April to 31 August 2016
11. Elisa Petranich, Department of Mathematics & Geosciences (DMG), Trieste, Italy, 15 May to 10 June 2016
12. Dr Dimitra Lambropoulou, University of Thessaloniki, Greece, 25 May 2016
13. Dr Miren Lopez deAlda, CSIC, Barcelona, Spain, 20 April 2016
14. Tolongutov Baigabyl, State Regulation Center on Environment Protection and Ecosafety of the SAEPP of Kyrgyz Republic, Bishkek, Kirgizistan, Mademinov Muradyl, Dzhogorku Kenesh of Kyrgyz Republic, Bishkek, Kirgizistan, Zhutanov Almaz, Dzhogorku Kenesh of Kyrgyz Republic, Bishkek, Kirgizistan, Kozhogulov Bakytbek, Project Research Organization Ken-Too, Kyrgyz Republic, Bishkek, Kirgizistan, Isakov Ilias, Khaidarkan Mercury Plant, Kyrgyz Republic, Batken region, Aidarken, Razakov Zhenish, Representative of Government in Batken region, Kyrgyz Republic, Batken, Kirgizistan, Saitov Azamat, Sharapov Zakir, Aidarken city hall, Kyrgyz Republic, Batken region, Aidarken, Kirgizistan, Timur Dosmambetov, State Regulation Center on Environment Protection and Ecosafety of the SAEPP of Kyrgyz Republic, Kirgizistan, Satyvaldiev Asylbek, Government Office of Kyrgyz Republic, Bishkek, Kirgizistan, Dzhuraev Saidolimzhon, Dzhogorku Kenesh of Kyrgyz Republic, Bishkek, Kirgizistan, Davis Kenneth, United Nations Environment Programme, Chemicals and Waste Branch, Geneva, Switzerland, 4 May 2016
15. Prof. Ivana Ivančev Tumbas, Aleksandra Tubić, University of Novi Sad, Novi Sad, Serbia, 2–3 June 2016
16. Mauro Paolini, Fondazione Edmund Mach Research and Innovation Centre - Department Food Quality and Nutrition Stable Isotope and Traceability, S.Michele all'Adige, Italy, 1–30 September 2016
17. Kyrilo Korychenskyi, Ukrainian Hydrometeorological Institute (UHMI), Kiev, Ukraine, 9–12 September 2016
18. Nataša Sarap, Vinča Institute of Nuclear Sciences, Laboratorija za zaštitu od zračenja i zaštitu životne sredine Vinča, Serbia, 5–15 September 2016
19. Dr Maria Bonsignore, Istituto per l'Ambiente Marino Costiero (IAMC-CNR), (Institute for Coastal Marine Environment), Fraz. Campobello di Mazara, Tp, Italy, 16 September to 5 October 2016
20. Dr Neda Vdović, Nevenka Mikac, Irena Jurina Tokić, Maja Ivanić, Mavro Lučić, Niko Bačić, Ruder Bošković Institute, Zagreb, Croatia, 23 September 2016
21. Prof. Ivana Ivančev Tumbas, University of Novi Sad, Novi Sad, Serbia, 23 September to 2 October 2016
22. Minja Bogunović, University of Novi Sad, Novi Sad, Serbia, 26 September to 7 October 2016
23. Yelizaveta Melnik, Department of Rare, Scattered and Radioactive Element Technology, Tomsk Polytechnic University, Tomsk, Russian Federation, 7–30 October 2016
24. Prof. Gabriel J Bowen, Geology & Geophysics Department, University of Utah, Salt Lake City, United States of America, 10–13 October 2016
25. Zoltán Kern, István Fórizs, György Czuppon, Tamás Mona, Hungarian Academy of Sciences, Budapest, Hungary, 10–11 October 2016
26. Dr Maria Ângela Menezes, CDTN/CNEN, Belo Horizonte, Brazil, 15–31 October 2016
27. Faisal J H H A Alabasey, Radiation Protection Department, Ministry of Health, Kuwait, Kuwait, 17 October to 16 November 2016
28. Delali Tulasi, University of Ghana, School of Nuclear and Allied Sciences, Legon, Accra, Ghana, 17 October to 31 December 2016
29. Dr Lata Gawade, CSIR-National Institute of Oceanography, Dona Paula-Goa, India, 2–4 November 2016
30. Prof. Arndt Schimmelmann, Indiana University, Department of Geological Sciences, USA, 5–11 December 2016
31. Dr Lesley Chesson, IsoForensics Inc., USA, 6–11 December 2016
32. Prof. Milena Jovašević Stojanović, Ivan Lazović, M.Sc., 12–15 December 2016,
33. Dr Miloš Davidović, Dušan Topalović, M.Sc., Vinča Institute of Nuclear Sciences, 12.–16. 12. 2016

## STAFF

### Researchers

1. Prof. Ljudmila Benedik
  2. Asst. Prof. Ingrid Falnoga
  3. Dr. David John Heath
  4. Prof. Ester Heath
  5. Prof. Milena Horvat, Head
  6. Dr. Radojko Jaćimović
  7. Asst. Prof. Zvonka Jeran
  8. Dr. David Kocman
  9. Asst. Prof. Branko Kontić
  10. Asst. Prof. Tina Kosjek
  11. Dr. Jože Kotnik
  12. Dr. Aleš Lapanje
  13. Prof. Sonja Lojen
  14. Dr. Darja Mazej
  15. Prof. Radmila Milačić
  16. Prof. Nives Ogrinc
  17. Prof. Borut Smodiš
  18. Prof. Janez Ščančar
  19. Asst. Prof. Zdenka Šlejkovec
  20. Dr. Marko Štrok
  21. Prof. Janja Vaupotič
  22. Dr. Polona Vreča
  23. Asst. Prof. Tea Zuliani
  24. Dr. Dušan Žigon
- Postdoctoral associates**
25. Dr. Marjeta Česen
  26. Dr. Tjaša Kanduč

27. Dr. Davor Kontić
  28. Dr. Kelly Peeters
  29. Dr. Tomaž Rijavec
  30. Dr. Miha Trdin
- Postgraduates**
31. Lojze Gačnik, B. Sc.
  32. Ana Jerše, B. Sc.
  33. Ana Kovačić, B. Sc.
  34. Ana Kroflič, B. Sc.
  35. Petra Novak, B. Sc.
  36. Majda Pavlin, B. Sc.
  37. Dr. Petra Planinšek, left 05.01.16
  38. Doris Potočnik, B. Sc.
  39. Johanna Amalia Robinson, B. Sc.
  40. Janja Snoj Tratnik, B. Sc.
  41. Anja Stajnko, B. Sc.
  42. Vanja Usenik, B. Sc.
  43. Janja Vidmar, B. Sc.
  44. Igor Živković, B. Sc.
- Technical officers**
45. Vesna Fajon, B. Sc.
- Technical and administrative staff**
46. Damjana Nikovski, B. Sc.
  47. Janja Smrke, retired 19.12.16
  48. Barbara Svetek, B. Sc.
  49. Zdenka Trkov, B. Sc.
  50. Stojan Žigon

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Enrica Alasonati *et al.* (11 authors), "Towards tributyltin quantification in natural water at the environmental quality standard level required by the water framework directive", *Talanta (Oxford)*, vol. 160, pp. 499-511, 2016.
2. Marina Arcagni, Andrea Rizzo, Romina Juncos, Majda Pavlin, Linda Campbell, Maria Arribére, Milena Horvat, Sergio Ribeiro Guevara, "Mercury and selenium in the food web of Lake Nahuel Huapi, Patagonia, Argentina", *Chemosphere (Oxford)*, vol. 166, pp. 163-173, 2016.
3. Karmen Bat, Klemen Eler, Darja Mazej, Branka Mozetič Vodopivec, Ines Mulič, Peter Kump, Nives Ogrinc, "Isotopic and elemental

- characterisation of Slovenian apple juice according to geographical origin: preliminary results", *Food chem.*, vol. 203, pp. 86-94, 2016.
4. Ermira Begu, Yaroslav Shlyapnikov, Andrej Stergaršek, Peter Frkal, Jože Kotnik, Milena Horvat, "A method for semi-continuous measurement of dissolved elemental mercury in industrial and natural waters", *Int. j. environ. anal. chem.*, vol. 96, iss. 7, pp. 609-626, 2016.
  5. Ljudmila Benedik, "Evaluation of procedures for Ra-226 determination in samples with high barium concentration by alpha-particle spectrometry", *Appl. radiat. isotopes*, vol. 109, pp. 210-213, 2016.
  6. Arne Bratkčič, Mitja Vahčić, Jože Kotnik, Kristina Obu, Ermira Begu, E. Malcolm S. Woodward, Milena Horvat, "Mercury presence and speciation in the South Atlantic Ocean along the 4023S transect", *Glob. biogeochem. cycles*, vol. 30, iss. 2, pp. 105-119, 2016.
  7. Mihael Brenčič, Polona Vreča, "Hydrogeological and isotope mapping of the karstic River Savica in NW Slovenia", *Environmental earth sciences*, vol. 75, nol. 8, pp. 651-1-651-13, 2016.
  8. Ivana Capan, Ž. Pastuović, R. Siegele, Radojko Jačimović, "Vacancy-related defects in n -type Si implanted with a rarefied microbeam of accelerated heavy ions in the MeV range", *Nucl. instrum. methods phys. res., B Beam interact. mater. atoms*, vol. 372, pp. 156-160, 2016.
  9. Marjeta Česen, Tina Eleršek, Matjaž Novak, Bojana Žegura, Tina Kosjek, Metka Filipič, Ester Heath, "Ecotoxicity and genotoxicity of cyclophosphamide, ifosfamide, their metabolites/transformation products and their mixtures", *Environ. pollut. (1987)*, vol. 210, pp. 192-201, 2016.
  10. Marjeta Česen, Tina Kosjek, Francesco Busetti, Boris Kompare, Ester Heath, "Human metabolites and transformation products of cyclophosphamide and ifosfamide: analysis, occurrence and formation during abiotic treatments", *Environ. sci. pollut. res. int.*, vol. 23, iss. 11, pp. 11209-11223, 2016.
  11. Marjeta Česen, Dimitra A. Lambropoulou, Maria Laimou-Geraniou, Tina Kosjek, Urška Blaznik, David John Heath, Ester Heath, "Determination of bisphenols and related compounds in honey and their migration from selected food contact materials", *J. agric. food chem.*, vol. 664, iss. 46, pp. 8866-8875, 2016.
  12. Romina Daga, Sergio Ribeiro Guevara, Majda Pavlin, Andrea Rizzo, Sonja Lojen, Polona Vreča, Milena Horvat, Maria Arribère, "Historical records of mercury in southern latitudes over 1600 years: Lake Futalufquen, Northern Patagonia", *Sci. total environ.*, vol. 553, pp. 541-550, 2016.
  13. Tadej Dolenc, Todor Serafimovski, Sonja Lojen, Matej Dolenc, Goran Tasev, Sabina Kramar, Nastja Rogan Šmuc, Petra Vrhovnik, "Environmental characterization of lake ecosystems located in Serbo Macedonian massif (FYRM)", In: *Biomaterialization: from fundamentals to biomaterials & environmental issues*, (Key Engineering Materials, Vol. 672), Frédéric Marin, ed., Pfaffikon, Trans Tech Publications, 2016, vol. 672, pp. 295-311, 2016.
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Jernej Jerman, Andrej Lešnjak, Luka Snoj, Borut Smodiš, "Inspection of the TRIGA reactor tank", In: *History, development and future of TRIGA research reactors*, (Technical report series, no. 482), Vienna, IAEA = International Atomic Energy Agency, 2016, 10 pp.
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## PATENT

1. Aleš Lapanje, *The impregnation process and attachment of microorganisms in porous materials*, SI24910 (A), Urad RS za intelektualno lastnino, 29. 07. 2016.

## MENTORING

1. Ermira Begu, *Determination of dissolved elemental mercury in surface and industrial waters*: doctoral dissertation, Ljubljana, 2016 (mentor Milena Horvat).
2. Marjeta Česen, *Occurrence, fate and effects of cytostatic residues in the aqueous environment*: doctoral dissertation, Ljubljana, 2016 (mentor Ester Heath; co-mentor Tina Kosjek).
3. Kristina Kotnik, *Occurrence, fate and toxicity of benzophenone derived compounds in the aqueous environment*: doctoral dissertation, Ljubljana, 2016 (mentor Ester Heath; co-mentor Tina Kosjek).
4. Petra Planinšek, *Plant uptake of selected natural radionuclides from contaminated environment*: doctoral dissertation, Ljubljana, 2016 (mentor Borut Smodiš; co-mentor Ljudmila Benedik).
5. Karmen Bizjak Bat, *Characterization of Slovenian apple juice with respect to its geographical origin and agricultural production practice*: doctoral dissertation, Nova Gorica, 2016 (mentors Nives Ogrinc, Branka Mozetič Vodopivec).
6. Katja Klun, *Composition and complexation of colloidal organic matter in coastal sea (Gulf of Trieste)*: doctoral dissertation, Ljubljana, 2016 (mentor Jadran Faganeli; co-mentor Ingrid Falnoga).
7. Sabina Berisha, *Mosses as bioindicators of trace elements and nitrogen in Ljubljana forest*: master's thesis, Ljubljana, 2016 (mentor Zvonka Jeran).
8. Dafina Kikaj, *Radon in soil gas in Kosovo*: master's thesis, Ljubljana, 2016 (mentor Peter Stegnar; co-mentors Zvonka Jeran, Meleq Bahtijari).
9. Hiacinta Klemenčič, *Priprava merilnih virov za spektrometrijo alfa s poudarkom na homogenosti nanosa*: master's thesis, Ljubljana, 2016 (mentor Helena Prosen; co-mentor Ljudmila Benedik).
10. Sebastijan Rep, *The role of spect/ct scintigraphy in localization of parathyroid adenomas*: master's thesis, Nova Gorica, 2016 (mentors Marko Hočevar, Janja Vaupotič).
11. Nataša Smrekar, *Assessment of effective doses based on various radon measuring techniques*: master's thesis, Nova Gorica, 2016 (mentor Janja Vaupotič).
12. Katja Valek, *Comparison analysis of formal air impact assessment in the procedure of environmental impact assessment with similar informal analysis performed by experts*: master's thesis, Ljubljana, 2016 (mentor Branko Kontič).
13. Andraž Lovšin, *Optimization of continuous measurement of biologically available fraction of mercury in water sample*: master's thesis, Ljubljana, 2016 (mentor Romana Marinšek Logar; co-mentor Aleš Lapanje).





# DEPARTMENT OF AUTOMATION, BIOCYBERNETICS AND ROBOTICS E-1

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*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 robot 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 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, reconfigurable robotic 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 numerous EU projects in the area of robotics and artificial intelligence, health, and space technologies. We are also active in transferring our research results into various applications through direct collaborations with industry. By maintaining a critical mass of researchers in all areas within one programme group, we have managed to foster exciting multidisciplinary projects.*

*Research in the area of humanoid and cognitive robotics as well as robot learning is primarily conducted within the Humanoid and Cognitive Robotics Lab (leader dr. Bojan Nemec), 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.*



Head:  
Prof. Aleš Ude

During the past year, our research focused on the development of cognitive robotic systems, new robot-learning methodologies, including imitation learning and autonomous exploration, contact modelling, humanoid robot vision, robotic assistive devices, reconfigurable robotic workcells, the automation of industrial manufacturing, studies of human physiology in extreme environments, an evaluation of protective equipment, and the development of biomedical methods. In the past year we acquired two new H2020 projects, AnDy (<http://www.andy-project.eu/>) and AUTOWARE (<http://www.autoware-eu.org>), and the programme GOSTOP, which is part of the smart specialization strategy of Slovenia and is coordinated by our department. Through these projects we will widen our research programme in the area of humanoid robotics and factories of the future.

## Robotics

In 2016 we continued our successful collaboration in the H2020 project ReconCell (A Reconfigurable robot workCell for the rapid set-up of automated assembly processes in SMEs, <http://www.reconcell.eu/>), where we developed new reconfiguration technologies that enable the rapid setup of robotic workcells in industrial production. The proposed workcell is based on a number of novel technologies including 1. robot programming by kinesthetic guiding, 2. sensor-based feedback control, 3. robot-aided reconfiguration, 4. object localization using 3-D vision, 5. visual quality control, 6. robot simulation, and 7. integration with business intelligence. Our software implementation is based on ROS (Robot Operating System), which provides tools for effective communications between all workcell elements. The main result in the past year was the development of new passive fixtures that can be automatically reconfigured by robotic manipulation. We developed new control techniques for automatic reconfiguration. Integration with robot-learning approaches based on kinesthetic guiding was also achieved.

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**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 the robotics and biomedical research is improving the quality of life.**

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Another important topic in the past year was the development of new methodologies for programming by the demonstration for bimanual tasks. This research was performed in the scope of the ARRS project “Learning and autonomous adaptation of dual arm assembly and service tasks”. We studied new representations for bimanual tasks based on a task decomposition into absolute and relative coordinates. A new approach where the human co-worker can modify both the spatial course of motion as well as the speed of execution in an intuitive way was developed. It allows a human co-worker to be less precise in the parts of the task that require high precision, as the precision aspect can be provided by the robot. The required dynamic capabilities of the robot were obtained by decoupling the bimanual robot dynamics in path operational space, which is attached to the desired trajectory.

**In EU project ACAT we developed a new methodology that enables statistical learning of compliant robot movements. For this purpose we applied a new movement representation called compliant movement primitives.**

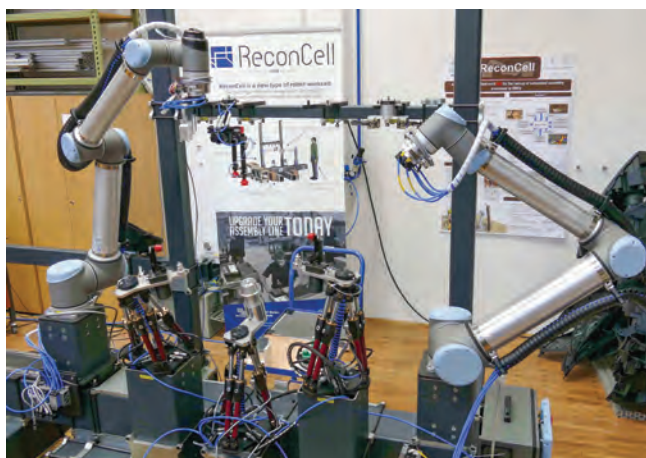


Figure 1: Reconfigurable robotic workcell

**Using a biologically plausible control method of an arm exoskeleton we extended the usable arm workspace where humans can efficiently perform manual operations.**



Figure 2: Reconfigurable fixture

Cognitive robots operating in natural environments should be able to quickly acquire new skills without extensive programming and mathematical modelling. In 2016 we successfully concluded the FP7 project ACAT (Learning and execution of action categories, <http://www.acat-project.eu/>). We showed that robot movements in contact with the environment can be effectively represented by position and orientation trajectories supplemented with the associated force-torque profiles. Statistical learning can be used for adaptation. To implement compliant robot movements when mathematical task models are not available, we extended the framework of **dynamic movement primitives** with **torque primitives**. The applicability of the proposed approaches was shown on several problems from automated assembly. Besides publications in high-quality international journals, we also presented the results of the ACAT project at the largest industrial fair in the world, Hannover Messe 2016.

In the scope of the Horizon 2020 project SPEXOR (<http://www.spexor.eu/>) we developed a **novel control approach** for robots that are **physically coupled with humans**, such as exoskeletons and assisting devices. In contrast with the conventional controllers, where assistance is usually provided indifferently of the configuration of the arm and direction of the motion, we propose a control method that compensates the **anisotropic property of the manipulability** related to the human arm. Consequently, the assistive behaviour of the proposed method allows the user to perform tasks in arm configurations that are otherwise unsuitable due to the lack of manipulability. In effect, the proposed method transforms the elliptical shape of the force manipulability ellipse to a circular shape in the whole space of human arm configurations. We evaluated the proposed approach by an experimental study where a group of subjects wearing a 2 DOF arm-exoskeleton had to move a 4 kg weight between several locations. The results of our study demonstrate that the proposed approach **effectively augments the ability of human motor control** to perform tasks equally well in the whole arm workspace that include configurations with a low intrinsic manipulability.

Many studies on human motor control have examined how humans move their arms. A well-known phenomenon called Fitts’ law describes the trade-off between the speed of motion and its accuracy. In robotics, many studies were performed and different control methods were proposed for robots working in well-structured environments. Nevertheless, the cooperation between humans and robots remains a challenging task that is highly relevant for **robots aiming to work together with humans in non-structured environments**. We developed a novel method for the on-line adaptation of robotic trajectories, where humans and robots are autonomous agents coupled through physical interaction, for example, through a manipulated object. Within the proposed framework, the robot adapts to the human motion through the sensory feedback by taking into account the Fitts’ law where the user-specific behaviour is estimated using a recursive least-square update. The movement trajectories are represented by the **dynamic movement primitives**, where the adaptation relies on the **iterative learning control** framework. The proposed approach was evaluated by a cooperative human-robot arm reaching task on a plane. We tested the accuracy and efficiency of the proposed method, showed its relevance and demonstrated that the proposed approach fully adapts to the human motor control and maintains the desired accuracy of the movement.

### Automation and industrial robotics

An important mission of our department is to transfer our research results to industrial applications. In the past year we prepared and launched a new program in the scope of Slovenia's smart-specialization strategy GOSTOP: Building blocks, tools and systems for factories of the future. The aim of the proposed GOSTOP program is to accelerate the development of the factories of the future concept in Slovenia and to provide solutions to the current needs of Slovenian industry, where some companies have already started to introduce this concept into their production facilities. In GOSTOP, 13 companies and 6 research organizations with compatible R&D programs in the factories of the future area joined forces to advance the concept. We identified 4 areas in which decisive breakthroughs can be achieved in Slovenia in the near future: **control technologies, tooling, robotics, and photonics**. In the area of robotics we collaborate with companies such as Kolektor, Domel, Yaskawa, and Podkrižnik.

Our main topics in GOSTOP program are: 1. **intelligent sensors and actuators**, 2. **adaptive robotic workcell for visual quality control**, and 3. **platform of the virtual factory**. Research in the area of intelligent sensors and actuators is directed towards the development of intelligent drive systems with torque-control algorithms and a built-in monitoring system and the possibility for predictive maintenance for each drive system. The second research theme, adaptive robotic workcell, will concentrate on new flexible grasping and manipulation processes, machine-vision, and machine-learning solutions. A specific objective of this activity is to develop an adaptive robotic workcell for the quality control of industrial parts. This will open new opportunities for robots in various tasks that are nowadays still done manually. The main goal of the platform of the virtual factory development is to design and produce an intelligent, competitive, sustainable information system in a smart factory that includes the elements of robotics. This will include research in the field of intelligent control algorithms, discrete event simulation in real time, and Plug & Produce interfaces with the principles of IoT.

### Environmental physiology and ergonomics

The **Biocybernetics group** in our department focuses primarily on research concerning the influence of extreme environmental factors on humans as well as on the development and evaluation of technology, and strategies to maintain safety and unhindered performance in such environments.

We maintain a research facility at the Nordic Centre Planica, where we conduct studies investigating the effect of **inactivity and unloading of the weight-bearing limbs** on physiological function. The effects of inactivity/unloading, as experienced by astronauts during microgravity exposure in space, is simulated with the bed-rest experimental model. Prolonged exposure to microgravity results in musculoskeletal atrophy and deconditioning of the cardiovascular system, which constitute a threat to the health and well-being of astronauts. Given that various space agencies are aiming to pursue long-term space mission in the near future, novel issues connected to space habitation are highly important. In particular, due to technical reasons, the environment within future Lunar and Mars habitats will be **hypobaric and hypoxic**. The continued aim of our research programme in space life sciences is to assess the effect of hypoxia on the processes of adaptation to microgravity which have been observed in a normoxic environment. We achieve this by comparing the adaptation of physiological systems to inactivity/unloading in a normoxic environment, with the changes observed in a hypoxic environment. Our current research in this area mostly focusses on novel strategies to counter the effects of inactivity and/or hypoxia on musculoskeletal system deconditioning.

We have initiated a research programme investigating the concept of physiological cross-tolerance. Specifically, we are investigating how prolonged exposure to one environmental stressor will influence the same responses to another stressor. We are currently most interested in the interactions between heat and hypoxia, their respective effects on human performance, and on the characteristics of autonomic temperature regulation. Another focus of our research is the effect of ambient humidity on thermal balance, physical performance, and cognitive function.

**We prepared and launched a new program in the scope of Slovenia's smart-specialization strategy GOSTOP: Building blocks, tools and systems for factories of the future.**



Figure 3: Robot programming by kinesthetic guiding

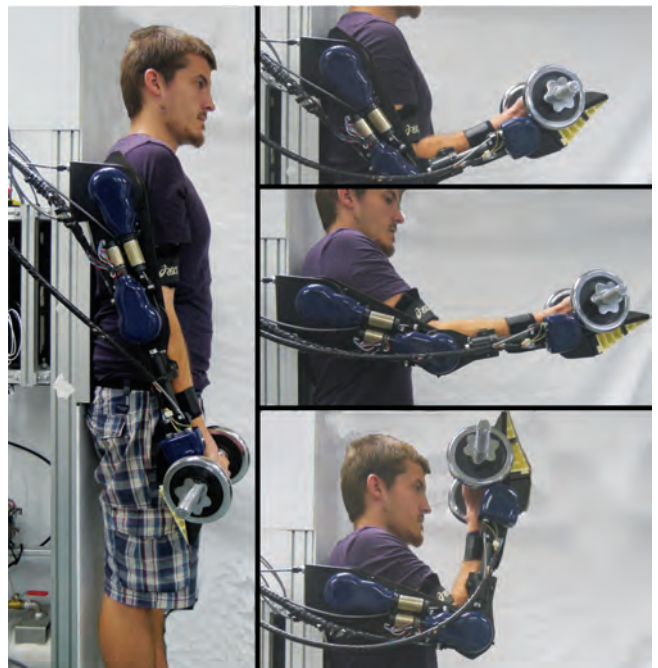


Figure 4: Weight manipulation supported by an exoskeleton



Figure 5: Investigating the effect of hypoxic acclimation on exercise performance in a hot environment

In this regard, we continue to assess the available technologies and various strategies in maintaining unhindered performance in hot environments.

With the industrial partner Kimberly-Clark (USA) we investigate novel strategies in the development of **optimal personal protective garments**. A significant step in our human manikin programme was the development of a **sweating thermal head manikin**, with both visual and breathing functionality. Visual images obtained from cameras situated in the eye sockets of the manikin can be analysed with dedicated software to provide an index of the magnitude of fogging in say goggles and/or face masks/visors. Furthermore, the mouth of the manikin is connected to a breathing simulator that monitors the pressure and volume during inspiration and expiration, and calculates the work of breathing imposed by a breathing apparatus. The sweating thermal head manikin is currently being used for evaluating helmets, hoods and breathing apparatus. Additionally, utilising our **sweating thermal hand manikin** we evaluated the thermal and evaporative resistances of new concepts in hand protection for the industrial partner W.L. Gore and Associates (USA & Germany).



Figure 6: Sweating thermal head manikin

Compression socks are now widely used in recreation, sport and rehabilitation. Standards have been established governing their classification and use, yet there is a paucity of data concerning their efficacy. In collaboration with industrial partner Intersocks d.o.o., we studied the **effect of applying compression socks** during recovery following a variety of activities in laboratory and field conditions. The results indicate that, though the magnitude of the exercise-induced delayed onset muscle soreness is reduced by the application of compression socks, the use of the socks does not exert any significant effect on subsequent muscle function.

Our hypoxic exercise and confinement studies investigate the potential additive effects of exercise training during intermittent or continuous exposure to hypoxia on appetite regulation, oxidative stress and sleep modulation. The impetus for these studies is recent evidence that **hypoxia per se can modify appetite** and thereby modulate body mass, and could thus provide a strategy for inducing weight loss and treating metabolic syndrome. 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 Europe, particularly among children and adolescents.

Physical disabilities are no longer a hindrance to participation in recreation and outdoor activities. Paraplegic individuals, for example, now practice diving with self-contained underwater breathing apparatus. In cooperation with personnel from the University Clinical Centre Maribor we investigated the effect of cold-water immersion on the physiological responses of paraplegic divers. In particular, we studied their ability to maintain their core temperature during a simulated dive protocol in cold water.



Figure 7: Testing of compression socks

With the support of the Slovenian Sport Foundation we investigated the **effect of simulated altitude conditions on factors** that can affect alpine skiing ability in children. Whereas in the past recreational skiing was limited to low altitudes, present day development of high-altitude ski resorts allows individuals of all ages and abilities to ascend to such high-altitude ski slopes (> 3000m). The altitude of such EU ski resorts is at a level where the prevailing hypoxia may have **detrimental effects** on a variety of physiological and psychological systems. We assessed the effect of hypoxia on: i) cardiorespiratory responses to exercise on a cycle and ski ergometer, ii) muscle strength, iii) orthostatic tolerance, iv) visual function, v) sleep, vi) pulmonary function, and vii) cognitive function. The study was conducted at our research facility at the Olympic Sport Centre Planica. There does not appear to be a significant difference between adults and children, in the manner and magnitude of the effect of hypoxia on physiological factors important for downhill skiing.

Hypoxia associated with high-altitude exposure triggers numerous **cardiovascular adjustments** and can lead to life-threatening conditions.

Nowadays a vast number of high altitude visitors are potentially more susceptible to the detrimental effects of **hypobaric hypoxia**. In particular, individuals born prematurely might be especially vulnerable due to prematurity induced cardiorespiratory control alternations resulting in **blunted ventilator and cerebrovascular responses to hypoxia**. Within the ARRS-funded project we compared the effect of normobaric and hypobaric hypoxic exercise-

induced cardiorespiratory responses in adults that had been born prematurely with results observed in normal-birth individuals. Preliminary data indicates that individuals born prematurely might exhibit reduced ventilatory response at rest, but not during physical activity.

Climate change is the biggest global health threat of the 21st century, with enormous consequences for humanity. Rising temperatures have been observed in Europe considerably more than in other areas, and have become a growing challenge for our community. Problems are already experienced by millions of Europeans during summer months, particularly in occupational settings. In addition to the well-known effects of heat exposure, a number of studies have confirmed a 2% reduction in productivity for each degree centigrade above 25°C. Given this productivity loss, **reducing the impacts of rising workplace temperatures** will produce two strategic benefits for EU: i) it will ensure the wellbeing of the EU's workforce, and ii) it will improve the EU's competitiveness and secure its future economy. In the framework of the Horizon 2020 project "Heat Shield" we are collaborating with the industrial partner Odello to mitigate the detrimental effects of heat waves on the workforce in their manufacturing plant.

### Some outstanding publications in the past years

1. J. Babič, E. Oztop, and M. Kawato (2016) Human motor adaptation in whole body motion. *Scientific Reports*, vol. 6, pp. 32868-1-32868-12.
2. M. Deniša, A. Gams, A. Ude, and T. Petrič (2016) Learning compliant movement primitives through demonstration and statistical generalization. *IEEE/ASME Transactions on Mechatronics*, vol. 21, no. 5, pp. 2581-2594
3. E. Rueckert, J. Čamernik, J. Peters, and J. Babič (2016) Probabilistic movement models show that postural control precedes and predicts volitional motor control. *Scientific Reports*, vol. 6, pp. 28455-1- 28455-12.
4. A. Gams, T. Petrič, M. Do, B. Nemeč, J. Morimoto, T. Asfour, and A. Ude (2016) Adaptation and coaching of periodic motion primitives through physical and visual interaction, *Robotics and Autonomous Systems*, vol. 75, pp. 340-351.
5. L. Peternel, T. Petrič, T. Noda, A. Ude, J. Morimoto, and J. Babič (2016) Adaptive control of exoskeleton robots for periodic assistive behaviours based on EMG feedback minimisation, *PLoS ONE*, vol. 11, no. 2, e0148942.
6. T. Debevec, E. J. Simpson, I. B. Mekjavić, O. Eiken, and I. A. Macdonald (2016) Effects of prolonged hypoxia and bed rest on appetite and appetite-related hormones. *Appetite*, vol. 107, pp. 28-37.
7. B. Mekjavić, M. Amon, R. Kölegård, S. N. Kounalakis, L. Simpson, O. Eiken, M. E. Keramidas, and I. A. Macdonald (2016) The effect of normobaric hypoxic confinement on metabolism, gut hormones, and body composition: promised and limitations. *Frontiers in Physiology*, vol. 7, pp. 202-1-202-13.
8. T. Debevec, V. Pialoux, S. Ehrström, A. Ribon, O. Eiken, I. B. Mekjavić, and G. P. Millet (2016) Femhab: the effects of bed rest and hypoxia on oxidative stress in healthy females. *Journal of Applied Physiology*, vol. 120, no. 8, pp. 930-938.

### Organization of conferences, congresses and meetings

1. 6th International Conference on the Physiology and Pharmacology of Temperature Regulation (PPTR), Ljubljana, 5. – 9. 12. 2016.
2. Workshop at European Robotics Forum (ERF 2016): Efficient Robot Programming, Force Control and Passive Reconfiguration Technologies for Fast Set-Up of Robotic Workcells, Ljubljana, 23. 3. 2016.
3. Workshop at a major robotics conference IROS 2016: Human-Robot Collaboration: Towards Co-Adaptive Learning Through Semi-Autonomy and Shared Control, Daejeon, Korea, 10. 10. 2016.
4. Kick-off meeting of Horizon 2020 project SPEXOR, Ljubljana, 28. – 29. 1. 2016.
5. General meeting of Horizon 2020 project ReconCell, Ljubljana, 10. – 20. 9. 2016.

## INTERNATIONAL PROJECTS

- |  |   |
|--|---|
| 1. Stimulators and Parts<br>Prof. Aleš Ude   | Prof. Aleš Ude<br>European Commission   |
| 2. Yaskawa: Polishing and Grinding by Programming by Demonstration and Autonomous Adaptation<br>Prof. Aleš Ude<br>Yaskawa Electric Corporation | 7. 7FP - CoDyCo; Whole-body Compliant Dynamical Contacts in Cognitive Humanoids<br>Asst. Prof. Jan Babič<br>European Commission   |
| 3. Kimberly-Clark - Development of LCD Shutter in the Year 2016<br>Asst. Prof. Leon Žlajpah<br>Kimberly-clark                                  | 8. COST CA16116 - 20786; Wearable Robots for Augmentation, Assistance or Substitution of Human Motor Functions<br>Asst. Prof. Jan Babič<br>Cost Office  |
| 4. Kimberly Clark: Stetson and Pillars of Comfort<br>Prof. Igor Mekjavić<br>Kimberly-clark   | 9. H2020 - HEAT-SHIELD; Integrated Inter-Sector Framework to increase the Thermal Resilience of European Workers in the Context of Global Warming<br>Prof. Igor Mekjavić<br>European Commission |
| 5. Yaskawa: Polishing and Grinding by Programming by Demonstration<br>Prof. Aleš Ude<br>Yaskawa Electric Corporation                           | 10. H2020 - AUTOWARE; Wireless Autonomous, Reliable and Resilient Production Operation Architecture for Cognitive Manufacturing   |
| 6. 7FP - ACAT; Learning and Execution of Action Categories   |   |

- Prof. Aleš Ude  
European Commission
11. H2020 - ReconCell; A Reconfigurable Robot Workcell for Fast Set-up of Automated Assembly Processes in SME-s  
Prof. Aleš Ude  
European Commission
  12. H2020 - SPEXOR; Spinal Exoskeletal Robot for Low Back Pain Prevention and Vocational Reintegration  
Asst. Prof. Jan Babič  
European Commission
  13. Control of Bimanual Physical Human-Robot Interaction for Rehabilitation and Industrial Services  
Asst. Prof. Andrej Gams  
Slovenian Research Agency
  14. Improving Prediction of Optimization Based Model-Predictive Control for High-Performance Bipedal Robotic Platforms with Learning of Initial Approximations  
Asst. Prof. Andrej Gams  
Slovenian Research Agency
  15. Discovery of the Optimality Criteria for Full Body Human Movements Using Inverse Reinforcement Learning  
Asst. Prof. Jan Babič  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Avtomation, robotics and biocybernetics  
Prof. Igor Mekjavič

## VISITORS FROM ABROAD

1. dr. Han Houdijk, Heliomare, Amsterdam, Netherlands 28 - 30 January 2016
2. dr. Coen van Bannek, Heliomare, Amsterdam, Netherlands 28 - 30 January 2016
3. Idsart Kingma, Vrije Universiteit, Amsterdam, Netherlands 28 - 30 January 2016
4. Jacob Hendrik Van Dieen, Amsterdam, Netherlands, 28. - 30 January 2016
5. prof. Ludovic Righetti, Max Planck Institute, Germany, 30 March - 2 April 2016
6. dr. Diane Cooper, DLR, Köln, Germany 14 - 28 February 2016
7. Prof. Egon Muller, Technische Universität Chemnitz, Chemnitz, Germany, 21-24 March 2016
8. Michael Koehle, University of British Columbia, Canada, 7 - 9 March 2016
9. Mathias Pousset, Centre Hospitalier Regional Universitaire de NANCY, Lausanne, Switzerland, 9 - 12. May 2016
10. prof. Mikael Grönkvist, KTH, Stockholm, Sweden, 29 March - 8 April 2016
11. prof. dr. Ola Eiken, KTH, Stockholm, Sweden, 29 March - 8 April 2016
12. dr. Mirko Raković, University of Novi Sad, Novi Sad, Serbia, 10 - 12 May 2016
13. dr. Srđan Savić, University of Novi Sad, Novi Sad, Serbia, 10 - 12 May 2016
14. dr. Milutin Nikolić, University of Novi Sad, Novi Sad, Serbia, 10 - 12 May 2016
15. Aleksandar Batinića, University of Novi Sad, Novi Sad, Serbia, 10 - 12 May 2016
16. prof. dr. Craig Asmundson, Univerza Simon Frazer, Vancouver, Canada, 12 -13 May 2016
17. Franck Buret, Kimberly Clark, Roswell, USA, 6 - 10 June 2016
18. Manish Raval, Kimberly Clark, Roswell, USA, 6 - 10 June 2016
19. Damon Larkin, Kimberly Clark, Roswell, USA, 6 - 10 June 2016
20. Lenox Wilson, Kimberly Clark, Roswell, USA, 6 - 10 June 2016
21. Pam Mayberry, Kimberly Clark, Roswell, USA, 3 - 11 June 2016
22. Stephanie Teat, Kimberly Clark, Roswell, USA, 3 - 11 June 2016
23. Roberto Greselin, Kimberly Clark, Roswell, USA, 8 - 9. June 2016
24. dr. Kai Salminen, Hermia Group New Factory Ltd, Tampere, Finland, 23 - 28 July 2016
25. Michael Kaplin, Eberhard Karls University Tuebingen, Dettingen, Germany, 3 October - 4 November 2016
26. Marc Piggemeyer, Institute for Man-Machine Interaction, RWTH Aachen University, Aachen, Germany, 28 August - 3. September 2016
27. Anders Prier Lindvig, University of Southern Denmark, Odense, Denmark, 12 - 20 September 2016
28. Prof. Ken Parsons, Loughborough University, Leicestershire, United Kingdom, 4.- 10. 12. 2016
29. Alex Buoite Stella, University of Udine, Udine, Italy, 4 - 9 December 2016
30. dr. Jessica Mee, Bangor University, Bangor, Gwynedd, United Kingdom, 4 - 9 December 2016
31. dr. Oliver Gibson, Brunel University, London, United Kingdom, 4 - 9 December 2016
32. dr. Yungbin Kim, Seoul National University, Seoul, South Korea, 4 - 10 December 2016
33. Sora Shin, Seoul National University, Seoul, South Korea, 3 - 9 December 2016
34. Panagiotis Miliotis, National and Kapodistrian University of Athens, Athens, Greece 4 - 10 December 2016

## STAFF

### Researchers

1. Asst. Prof. Jan Babič
2. Asst. Prof. Tadej Debevec
3. Asst. Prof. Andrej Gams
4. Asst. Prof. Igor Kovač
5. Prof. Igor Mekjavič
6. Asst. Prof. Bojan Nemeč
7. Dr. Matjaž Omladič
8. Dr. Tadej Petrič
9. Asst. Prof. Dušan Ponikvar\*
10. Dr. Anton Ružič
11. **Prof. Aleš Ude, Head**
12. Asst. Prof. Leon Žlajpah

### Postdoctoral associates

13. Dr. Urša Ciuha
14. Prof. Igor Klep
15. Prof. Tomaž Košir\*
16. Asst. Prof. Marjeta Kramar Fijavž\*
17. Dr. Nejc Likar
18. Dr. Adam Mc Donnell
19. Dr. Zrinka Potočanac
20. Dr. Barry Martin Ridge
21. Asst. Prof. Klemen Šivic\*
22. *Dr. Rok Vuga, left 01.06.16*

## R & D GRANTS AND CONTRACTS

1. Learning and autonomous adaptation of dual arm assembly and service tasks  
Prof. Aleš Ude
2. Cardiorespiratory responses during hypoxic exercise in individuals born prematurely  
Asst. Prof. Tadej Debevec
3. Methods of algebra and functional analysis in theory and practice of financial mathematics  
Prof. Igor Klep
4. Building blocks, tools and systems for the Factories of the Future - GOSTOP  
Asst. Prof. Igor Kovač
5. Customer Service - Abroad  
Prof. Igor Mekjavič

## NEW CONTRACTS

1. Specification of requirements and development of solutions for an automatic MES, supervision and plant control system  
Dr. Anton Ružič  
Žito Prehrambena Industrija, d. d.
2. Prevention of delayed onset muscle soreness using compression socks  
Prof. Igor Mekjavič  
Intersocks d. o. o., Kočevje

### Postgraduates

23. Robert Bevec, B. Sc.
24. Jernej Camernik, B. Sc.
25. Miha Deniša, B. Sc.
26. Miha Dežman, B. Sc.
27. Timotej Gašpar, B. Sc.
28. Rok Goljat, B. Sc.
29. Aljaž Kramberger, B. Sc.
30. Rok Pahič, B. Sc.
31. Martin Pečar, B. Sc.
32. Alexandros Sotiridis, B. Sc.

### Technical officers

33. Martin Bem, B. Sc.
34. Mišel Cevzar, B. Sc.
35. Damjan Fink
36. Simon Reberšek, B. Sc.
37. Bogomir Vrhovc, B. Sc.

### Technical and administrative staff

38. Tanja Dragojevič, B. Sc.
39. *Anja Gosar, 01.12.16, transferred to Department U1*
40. Marija Kavčič, B. Sc.
41. Jana Stanič
42. Danijela Zeljković Anžiček, B. Sc.

Note:

\* part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Jan Babič, Erhan Oztop, Mitsuo Kawato, "Human motor adaptation in whole body motion", *Scientific reports*, vol. 6, pp. 32868-1-32868-12, 2016.
2. Urška Ciuha, Mikael Grönkvist, Igor B. Mekjavič, Ola Eiken, "Strategies for increasing evaporative cooling during simulated desert patrol mission", *Ergonomics*, vol. 59, no. 2, pp. 298-309, 2016.
3. Urška Ciuha, Igor B. Mekjavič, "Regional thermal comfort zone in males and females", *Physiol. behav.*, vol. 161, pp. 123-129, 2016.
4. Jernej Čamernik, Zrinka Potočanac, Luka Peternel, Jan Babič, "Holding a handle for balance during continuous postural perturbations: immediate and transitional effects on whole body posture", *Front. hum. neurosci.*, vol. 10, pp. 486-1-486-8, 2016.
5. Tadej Debevec, Vincent Pialoux, Sabine Ehrström, Alexandra Ribon, Ola Eiken, Igor B. Mekjavič, Grégoire P. Millet, "FemHab: the effects of bed rest and hypoxia on oxidative stress in healthy females", *J Appl Physiol*, vol. 120, no. 8, pp. 930-938, 2016.
6. Tadej Debevec, Elizabeth J. Simpson, Igor B. Mekjavič, Ola Eiken, Ian A. Macdonald, "Effects of prolonged hypoxia and bed rest on appetite and appetite-related hormones", *Appetite*, vol. 107, pp. 28-37, 2016.
7. Miha Deniša, Andrej Gams, Aleš Ude, Tadej Petrič, "Learning compliant movement primitives through demonstration and statistical generalization", *IEEE/ASME trans. mechatron.*, vol. 21, no. 5, pp. 2581-2594, 2016.
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9. Helio Fernandez Tellez, Shawnda A. Morrison, X Neyt, O. Mairesse, Maria Francesca Piacentini, E Macdonald-Nethercott, Andrej Pangerc, Leja Dolenc-Grošelj, Ola Eiken, Nathalie Pattyn, Igor B. Mekjavič, Romain Meeusen, "Exercise during short-term and long-term continuous exposure to hypoxia exacerbates sleep-related periodic breathing", *Sleep (New York)*, vol. 39, iss. 4, pp. 773-783, 2016.
10. Andrej Gams, Tadej Petrič, Martin Do, Bojan Nemeč, Jun Morimoto, Tamim Asfour, Aleš Ude, "Adaptation and coaching of periodic motion primitives through physical and visual interaction", *Robot. auton. syst.*, vol. 75, part B, pp. 340-351, 2016.
11. Polona Jaki, Eva Lenassi, Ola Eiken, Igor B. Mekjavič, "Effect of acute hypercapnia during 10-d hypoxic bed rest on posterior eye structures", *J Appl Physiol*, vol. 120, no. 10, pp. 1241-1248, 2016.
12. Michail E. Keramidas, Roger Kölegård, Igor B. Mekjavič, Ola Eiken, "PlanHab: hypoxia exaggerates the bed-rest-induced reduction in peak oxygen uptake during upright cycle ergometry", *Am J Physiol Heart Circ Physiol*, vol. 311, no. 2, pp. H453-H464, 2016.
13. Michail E. Keramidas, Igor B. Mekjavič, Roger Kölegård, Alexander Choukèr, Claudia Strewé, Ola Eiken, "PlanHab: hypoxia counteracts the erythropoietin suppression, but seems to exaggerate the plasma volume reduction induced by 3 weeks of bed rest", *Physiol. reports*, vol. 4, no. 7, pp. e12760-1-e12760-10, 2016.
14. Michail E. Keramidas, Nektarios Stavrou, Stylianos N. Kounalakis, Ola Eiken, Igor B. Mekjavič, "Severe hypoxia during incremental exercise to exhaustion provokes negative post-exercise affects", *Physiol. behav.*, vol. 156, pp. 171-176, 2016.
15. Igor Klep, Scott McCullough, Christopher Nelson, "On trace-convex noncommutative polynomials", *Mich. math. j.*, vol. 65, iss. 1, pp. 131-146, 2016.
16. Aljaž Kramberger, Rok Piltaver, Bojan Nemeč, Matjaž Gams, Aleš Ude, "Learning of assembly constraints by demonstration and active exploration", *Ind. rob.*, vol. 43, no. 5, pp. 524-534, 2016.
17. Polona Kraner Zrim, Igor B. Mekjavič, Tatjana Rijavec, "Properties of laminated silica aerogel fibrous matting composites for footwear applications", *Tex. res. j.*, vol. 86, no. 10, pp. 1063-1073, 2016.
18. Tijs Louwies, Polona Jaki, Bianca Cox, Ola Eiken, Igor B. Mekjavič, Stylianos N. Kounalakis, Patrick De Boever, "Separate and combined effects of hypoxia and horizontal bed rest on retinal blood vessel diameters", *Invest. ophthalmol. visual sci.*, vol. 57, no. 11, pp. 4927-4932, Sep. 2016.
19. Igor B. Mekjavič, Mojca Amon, Roger Kölegård, Stylianos N. Kounalakis, Liz Simpson, Ola Eiken, Michail E. Keramidas, Ian A. Macdonald, "The effect of normobaric hypoxic confinement on metabolism, gut hormones, and body composition: promised and limitations", *Front. physiol.*, vol. 7, pp. 202-1-202-13, 2016.
20. Grégoire P. Millet, Tadej Debevec, Franck Brocherie, Davide Malatesta, Oliver Girard, "Therapeutic use of exercising in hypoxia: promises and limitations", *Front. physiol.*, vol. 7, art. 224, 2016.
21. Shawnda A. Morrison, Andrej Pangerc, Ola Eiken, Igor B. Mekjavič, Leja Dolenc-Grošelj, "Effect of exercise on night periodic breathing and loop gain during hypoxic confinement", *Respirology*, vol. 21, iss. 4, pp. 746-753, May 2016.
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24. Zrinka Potočanac, Mirjam Pijnappels, Sabine Verschueren, Jaap van Dieën, Jacques Duysens, "Two stage muscle activity responses in decisions about leg movement adjustments during trip recovery", *Journal of neurophysiology*, vol. 115, no. 1, pp. 143-156, 2016.
25. Alexandra Ribon, Vincent Pialoux, Jonas J. Saugy, Thomas Rupp, Raphael Faiss, Tadej Debevec, Grégoire P. Millet, "Exposure to hypobaric hypoxia results in higher oxidative stress compared to normobaric hypoxia", *Respiratory physiology & neurobiology*, vol. 233, pp. 23-27, 2016.
26. Joern Rittweger *et al.* (11 authors), "On the combined effects of normobaric hypoxia and bed rest upon bone and mineral metabolism: results from the PlanHab study", *Bone*, vol. 91, pp. 130-138, 2016.
27. Elmar Rueckert, Jernej Čamernik, Jan Peters, Jan Babič, "Probabilistic movement models show that postural control precedes and predicts volitional motor control", *Scientific reports*, vol. 6, pp. 28455-1- 28455-12, 2016.
28. Erik Rullman, Igor B. Mekjavič, Helene Fischer, Ola Eiken, "PlanHab PlanHab (Planetary Habitat Simulation): the combined and separate effects of 21 days bed rest and hypoxic confinement on human skeletal muscle miRNA expression", *Physiol. reports*, vol. 4, no. 8, pp. e12753-1-e12753-12, 2016.
29. Elizabeth J. Simpson, Tadej Debevec, Ola Eiken, Igor B. Mekjavič, Ian A. Macdonald, "PlanHab: the combined and separate effects of 16 days bed rest and normobaric hypoxic confinement on circulating lipids and indices of insulin sensitivity in healthy men", *J Appl Physiol*, vol. 120, no. 8, pp. 947-955, 2016.
30. Pablo Ramon Soria, Robert Bevec, Begoña C. Arrue, Aleš Ude, Anibal Ollero, "Extracting objects for aerial manipulation on UAVs using low cost stereo sensors", *Sensors*, vol. 16, no. 5, pp. 700-1-700-19, 2016.
31. Rok Vuga, Bojan Nemeč, Aleš Ude, "Speed adaptation for self-improvement of skills learned from user demonstrations", *Robotica (Camb.)*, vol. 34, no. 12, pp. 2806-2822, 2016.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Miha Deniša, Aleš Ude, "Movement recognition and cooperative task synthesis through hierarchical database search", In: *Papers*, 25th International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2016, June 30th - July 2nd 2016, Belgrade, 7 pp.
2. Miha Deniša, Aleš Ude, Andrej Gams, "Adaptation of motor primitives to the environment through learning and statistical generalization", In: *Advances in robot design and intelligent control: proceedings of the 24th International Conference on Robotics in Alpe-Adria-Danube Region, (RAAD), [27-29 May 2015, Bucharest, Romania]*, (Advances in intelligent systems and computing, volume 371), pp. 449-457.
3. Miha Dežman, Tadej Debevec, Jan Babič, Andrej Gams, "Effects of passive ankle exoskeleton on human energy expenditure: pilot evaluation", In: *Papers*, 25th International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2016, June 30th - July 2nd 2016, Belgrade, 8 pp.
4. Miha Dežman, Tadej Debevec, Jan Babič, Andrej Gams, "Passive ankle exoskeleton: design and practical evaluation", In: *Zbornik*, 8. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana, 31. maj in 1. junij 2016, Ljubljana, Slovenija, pp. 140-148.
5. Andrej Gams, Tadej Petrič, "On-line modifications of robotic trajectories: learning, coaching and force vs. position feedback", In:



- Papers*, 25th International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2016, June 30th - July 2nd 2016, Belgrade, 8 pp.
6. Andrej Gams, Aleš Ude, "On-line coaching of robots through visual and physical interaction: analysis of effectiveness of human-robot interaction strategies", In: *ICRA 2016*, 2016 IEEE International Conference on Robotics and Automation, May 16-21, 2016, Stockholm, Sweden, pp. 3028-3034.
  7. Aljaž Kramberger, Andrej Gams, Bojan Nemec, Casper Schou, Dmimitros Chrysostomou, Ole Madsen, Aleš Ude, "Transfer of contact skills to new environmental conditions", In: *HUMANOIDS 2016*, IEEE-RAS 16th International Conference on Humanoid Robots, November 15-17, 2016, Cancun, Mexico, pp. 668-675.
  8. Aljaž Kramberger, Andrej Gams, Bojan Nemec, Aleš Ude, "Generalization of orientational motion in unit quaternion space", In: *HUMANOIDS 2016*, IEEE-RAS 16th International Conference on Humanoid Robots, November 15-17, 2016, Cancun, Mexico, pp. 808-813.
  9. Aljaž Kramberger, Casper Schou, Dmimitros Chrysostomou, Andrej Gams, Ole Madsen, Aleš Ude, "Fast setup and adaptation of industrial assembly tasks with force-based exception strategies: pilot evaluation", In: *Papers*, 25th International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2016, June 30th - July 2nd 2016, Belgrade, 8 pp.
  10. Igor B. Mekjavić, "Kampus Planica: predstavitev raziskovalnih del in dobre prakse: research and best practices", In: *Zbornik*, IX. konferenca slovenskih znanstvenikov in gospodarstvenikov iz sveta in Slovenije, Ljubljana, 27.-28. oktober 2016, pp. 134-136.
  11. Bojan Nemec, Nejc Likar, Andrej Gams, Aleš Ude, "Bimanual human robot cooperation with adaptive stiffness control", In: *HUMANOIDS 2016*, IEEE-RAS 16th International Conference on Humanoid Robots, November 15-17, 2016, Cancun, Mexico, pp. 607-613.
  12. Luka Peternel, Erhan Oztop, Jan Babič, "A shared control method for online human-in-the-loop robot learning based on locally weighted regression", In: *IROS 2016*, 2016/IEEE/RSJ International Conference on Intelligent Robots and Systems, September 28 - October 9-14, 2016, Daejeon, Korea, pp. 3900-3906.
  13. Tadej Petrič, Andrej Gams, "Effect of sequence order on autonomous robotic database expansion", In: *Papers*, 25th International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2016, June 30th - July 2nd 2016, Belgrade, 8 pp.
  14. Tadej Petrič, Rok Goljat, Jan Babič, "Augmentation of human arm motor control by isotropic force manipulability", In: *IROS 2016*, 2016/IEEE/RSJ International Conference on Intelligent Robots and Systems, September 28 - October 9-14, 2016, Daejeon, Korea, pp. 696-701.
  15. Tadej Petrič, Rok Goljat, Jan Babič, "Cooperative human-robot control based on Fitts' law", In: *HUMANOIDS 2016*, IEEE-RAS 16th International Conference on Humanoid Robots, November 15-17, 2016, Cancun, Mexico, pp. 345-350.
  16. Tadej Petrič, Aleš Ude, Auke Jan Ijspeert, "Autonomous learning of internal dynamic models for reaching tasks", In: *Advances in robot design and intelligent control: proceedings of the 24th International Conference on Robotics in Alpe-Adria-Danube Region, (RAAD), [27-29 May 2015, Bucharest, Romania]*, (Advances in intelligent systems and computing, volume 371), pp. 439-447.
  17. Barry Ridge, Aleš Ude, "Action-grounded surface geometry and volumetric shape feature representations for object affordance prediction", In: *HUMANOIDS 2016*, IEEE-RAS 16th International Conference on Humanoid Robots, November 15-17, 2016, Cancun, Mexico, pp. 1022-1028.
  18. Aleš Ude, Rok Vuga, Bojan Nemec, Jun Morimoto, "Trajectory representation by nonlinear scaling of dynamic movement primitives", In: *IROS 2016*, 2016/IEEE/RSJ International Conference on Intelligent Robots and Systems, September 28 - October 9-14, 2016, Daejeon, Korea, pp. 4728-4735.
  19. Adam Wolniakowski *et al.* (13 authors), "Optimizing grippers for compensating pose uncertainties by dynamic simulation", In: *SIMPAR proceedings*, 2016 IEEE International Conference on Simulation, Modeling, and Programming for Autonomous Robots, Dec. 13-16, San Francisco, USA, 8 pp.
  20. Tomaž Zavrl, Žiga Gosar, Igor Kovač, Aleš Ude, "Robotsko nalaganje kosov na plošče za planete za vakuumsko oslojevanje", In: *Vir znanja in izkušenj za stroko: zbornik foruma*, [8.] industrijski forum IRT, Portorož, 6. in 7. junij 2016, pp. 51-55.
  21. Leon Žlajpah, "Kinematic control of redundant robots in changing task space", In: *Papers*, 25th International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2016, June 30th - July 2nd 2016, Belgrade, 8 pp.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Miha Deniša, Tadej Petrič, Andrej Gams, Aleš Ude, "A review of compliant movement primitives", In: *Robot control*, Efrén Gorrostieta Hurtado, ed., Rijeka, InTech, 2016, pp. 1-17.

# DEPARTMENT OF SYSTEMS AND CONTROL

E-2

*The department is engaged in the analysis, control and optimization of systems and processes. The activities of the department are focused on the research of new methods and algorithms for automatic control, the development of procedures and tools to support the design 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 2016 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 first topic addressed the modelling and identification of nonlinear and complex dynamical systems. The research on methods for the dynamical systems' modelling was pursued in two directions: the development of Gaussian-process models and the development of model-tree ensembles. The research of modelling methods for environmental systems continued in the first track. In addition, a scientific monograph on modelling and control with Gaussian process models, authored by a member of department, was published by the Springer publishing house in 2016. The research of methods based on model-tree ensembles was focused on multivariable systems and on a comparison with other modelling methods.

The second topic was *advanced control*. We have continued the research and development of model predictive control (MPC) by using fast, online, first-order quadratic programming optimization techniques. Using singular value decomposition we have implemented an advanced MPC controller for the ITER plasma current and shape controller for the plasma magnetic control of the Iter fusion tokamak reactor, evaluated its simulation performance, and tested its numerical implementation in a low-latency Linux environment. Using an active-set approach, a new theoretical result on tight local convergence estimates was found for the dual gradient method, which explains different convergence rates observed in numerical simulations (Figure 1).

In the field of *fault detection and condition monitoring* our work included research dealing with robust fault detection in model-based approaches. In order to facilitate robust fault detection, we proposed a novel approach that combines elements of Gaussian process models and Jensen-Reny divergence. A Gaussian process model is employed in order to correct modelling errors due to a mismatch between measurements and a physical model employed for residual generation. Then, the residuals generated by employing physical and Gaussian models, are evaluated via Jensen-Reny divergence. The proposed approach was applied for SOFC fault detection and the results were presented at the *SysTOL* conference in Barcelona, Spain. The accurate anticipation of the remaining useful life (RUL) of a machine is also becoming mandatory in Industry 4.0 for efficient exploitation of the assets and avoiding unplanned downtimes. A novel, three-stage, data-driven approach to the RUL prediction has been developed and demonstrated on an industrial sand-blasting machine.

In 2016 we continued working on the diagnostics of PEM fuel cells with the use of its own developed fast electrochemical impedance spectroscopy. During the past 5 years we have achieved a considerable number of research and applied results in the area of PEM fuel-cell diagnostics. In 2016, all these results have been presented in a book, which is currently in the publishing process with the Springer publishing company.

In the area of **tools and building blocks for implementation** we have started the activities to upgrade the tool for analysis and optimisation of the production performance – ProOpter. We have overviewed current global initiatives and trends in the field of smart manufacturing. The main focus was to review functional and integrational aspects of the tool within the smart manufacturing ecosystem. Furthermore, architectural aspects were reviewed in order to be in line with the trends of Industry 4.0 (IoT, cloud, etc.) (Figure 2).

In the past year, a number of members of the department in collaboration with colleagues from other partner organisations, worked intensively on preparing a proposal for the public call entitled "Promoting the implementation of research and development programs (TRL 3-6)." We proposed



Head:

**Dr. Vladimir Jovan**

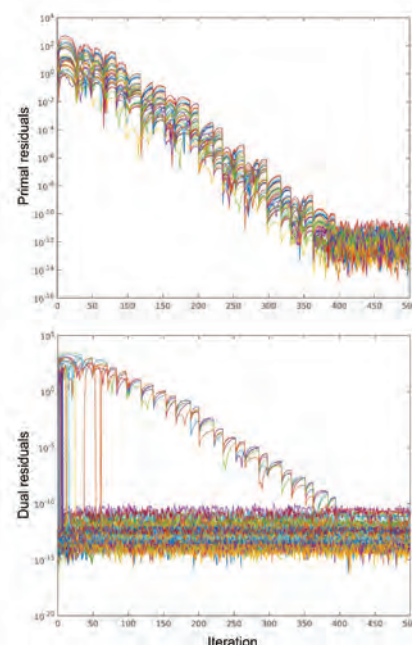


Figure 1: Convergence courses of primal (top) and dual (bottom) residuals through iterations of the dual fast gradient method with restarting at the optimization of a sample quadratic program of the plasma current and shape controller in one time-step. Validation of ozone-model predictions with measurements of maximum daily values

a program entitled "Building Blocks, tools and systems for factories of the future", with the acronym GOSTOP, in the frame of the priority area Factories of the Future. The application was successful and the work on the program started in November. The program will last 42 months, until end of April 2020. The program involves 19 partners, of which there are 6 institutions and 13 companies. The program is structured in two ways, first of which is based on the content, and second on the technology readiness level (TRL). In terms of content, the program is divided into four pillars, namely Control technologies, Tooling technology, Robotics, and Photonics. According to TRL, each

of the four pillars is divided into two research and development projects, of which first aims to achieve TRL 3-4 (industrial research), and second TRL 5-6 (experimental development). Hence, the program contains eight R&D projects. Members of our department are involved in the research and development activities of the program (in the Control technologies pillar), as well as in the program-management activities (deputy coordinator, member of the executive committee, chairman of the committee for the dissemination and exploitation of results, assistant of the program coordinator for R&D coordination, management of the Control technologies pillar, management of two activities of the Control technologies pillar).

Applied research in the priority problem domains was the third sub-area of our interest. In collaboration with SME Entia d.o.o. we completed Slovenian Research Agency project "Cost optimization of energy consumption for refrigeration in shopping malls," where we have developed a control system for freezers, which implicitly takes into account the prescribed temperature constraints according to the HACCP standard. The system simultaneously allows an adjustment of the total power consumption to the desired consumption profile.

For another on-going Slovenian Research Agency project named Development and implementation of a method for on-line modelling and forecasting

of air pollution research on algorithms for modelling and prediction based on Gaussian process that can be used with a mobile station were pursued. Moreover, the research was also pursued on empirical modelling methods for improved modelling and forecasting pollution with ozone over Slovenia as a case study of complex terrain.

In the past year a new test rig for electronically commutated motors has been set up in Domel d.o.o. For this purpose a new graphical user interface for the control and monitoring of motor parameters has been developed. The test system has been connected to the information system in Domel d.o.o. in line with Industry 4.0 trends. In addition, a new instrument has been prepared for monitoring the vibrations of motors with MEMS accelerometers. The purpose of the instrument is to explore possible ways of mounting MEMS accelerometers on existing electronically commutated motors and determine whether the installation of the MEMS sensors is economically justified.

Within the new project L2-7663 "State-of-health estimation of electrochemical energy systems", funded by Slovenian Research Agency, we were studying various models that describe the degradation phenomena in PEM fuel cells. For that purpose we have built a test-bench for run-to-failure testing of PEM fuel cells under various operating conditions.

### International R&D projects

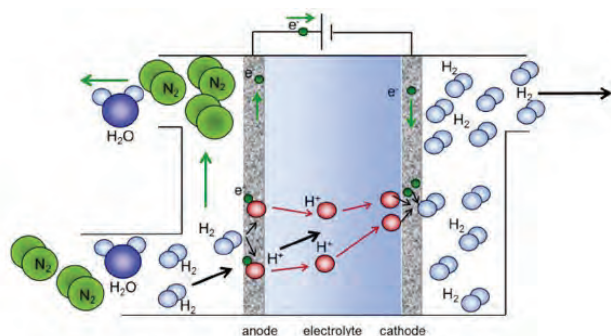
Since April 2014 we have participated in the third EU FW7 project "Diamond - Diagnosis-aided control for SOFC power systems". A simple, model-free supervisory optimizer for SOFC (solid-oxide fuel cell) power systems was designed. The optimizer adjusts set-points for the low-level controllers in such a way as to maximize the electrical efficiency of the system and prevent stack voltage drops. The optimization problem is solved by using the extremum-seeking approach where the optimum is sought directly on the process. The optimizer shows encouraging performance and exceeds the weakness of model-based optimizers, which assume nominal process conditions all the time and do not take into account the degradation process.

In the framework of the 3-year project "Fast Model Predictive Control for Magnetic Plasma Control - FMPCFMP", "Enabling Research" activity of the EUROfusion Work Programme 2015 (part of Horizon 2020 / Euratom), we have been collaborating with the consortium ENEA/CREATE from Naples, Italy. 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.



Figure 2: Smart Manufacturing Ecosystem

Figure 3: The principle of electro-chemical hydrogen compression and purification



At the beginning of 2017 a new H2020 hydrogen technology related project has been started where the Department of Systems and Control acts as a partner. The scope of the project is the development of an electro-chemical system for hydrogen compression and cleaning using membranes, similar to the ones used in PEM fuel cells. The compression system reaches pressure up to 1000 bar, it is driven by the electricity and it has higher energy efficiency than mechanical compressors. During decompression a part of the electrical energy utilized during compression is recuperated. The system can also be used for hydrogen cleaning since the membrane only conducts hydrogen protons (Figure 3).

Recent accomplishments in the health monitoring of solid-oxide fuel cells have given a boost to extending the methodology to a perspective technology of solid-oxide electrolyzers. The first step within a bilateral project with a French research institution CEA and our department, initiated in July 2016, was oriented towards a detailed feasibility study.

Within the COST Water\_2020 project we have participated in the preparation of the book chapter "Model-based comparative assessment of innovative processes". The objective of the chapter is to compare the simulation results of three different wastewater-treatment-plant configurations using dynamic modelling. The chapter is part of the book "Innovative Wastewater Treatment & Resource Recovery Technologies: Impacts on Energy, Economy and Environment" which is prepared by the partners of the COST Action. The book, which has more than 160 contributors, will be released by the IWA Publishing in May 2017.

#### Applied work

In the context of a long-term partnership with Danfoss Trata d.o.o in 2016 we started with the activities on the development of hardware and software for three new families of valve drives. There are various types and sizes of drives with a variety of functionalities to be used by both the HVAC systems as well as in district heating systems.

In Domel d.o.o. in 2016 the partial installation of a new diagnostic system for the end control of electronically commutated motors (type 771) has been completed. The system is based upon diagnostic systems on older production lines. Nevertheless, many innovations were introduced during the implementation on the electro-mechanical part as well as on the software part. The new system supports the diagnostics of two different motors, wherein one type of motor has a built-in controller, which further increases the complexity of manipulators and electronic components of the line (Figure 4). Next, on the software side the focus was on informatization of the production line in accordance with the current trend Industry 4.0 (IIoT – Industrial Internet Of Things). Thus, the majority of components and sensors has its own IP address and can communicate with the ERP system. The production line is scheduled to start operating in the first quarter of 2017.

Another project in Domel d.o.o was installed in their unit PE ECS. We have developed and installed a configurable end-quality control line for electronically commutated blowers. The line is capable of self-reconfiguration, thus enabling total end-quality control of all the produced blower families. The line's design and implementation is completely in line with Industry 4.0 guidelines.

#### 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 four Ph.D. students.

#### Some outstanding publications in the past year

1. Dolanc, Gregor, Pregelj, Boštjan, Petrovčič, Janko, Pasel, Joachim, Kolb, Günter. Control of autothermal reforming reactor of diesel fuel. *Journal of power sources*, ISSN 0378-7753, may 2016, vol. 313, pp. 223-232

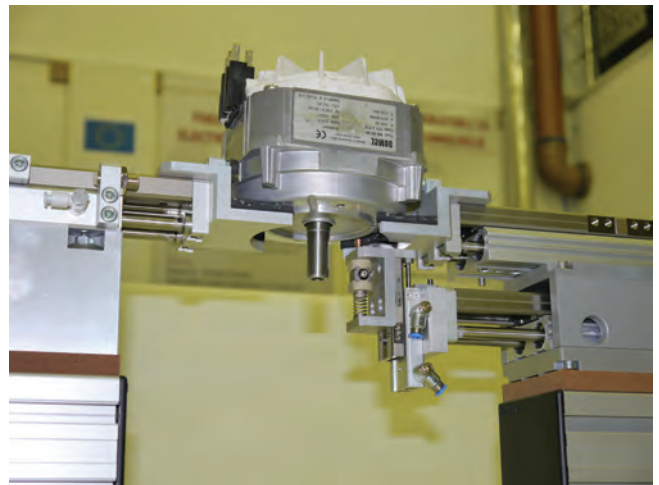


Figure 4: Gripper of the new system for the motor final quality control in Domel d.o.o.



Figure 5: Bowling tournament to celebrate the department's 30th anniversary

2. Nerat, Marko, Vrančič, Damir. A novel fast-filtering method for rotational speed of the BLDC motor drive applied to valve actuator. *IEEE/ASME transactions on mechatronics*, ISSN 1083-4435, 2016, vol. 21, no. 3, pp. 1479-1486
3. Dolenc, Boštjan, Vrečko, Darko, Juričič, Dani, Pohjoranta, Antti, Pianese, Cesare. Online estimation of internal stack temperatures in solid oxide fuel cell power generating units. *Journal of power sources*, ISSN 0378-7753, 2016, vol. 336, pp. 251-260
4. Pregelj, Boštjan, Micor, Michał, Dolanc, Gregor, Petrovčič, Janko, Jovan, Vladimir. Impact of fuel cell and battery size to overall system performance - a diesel fuel-cell APU case study. *Applied energy*, ISSN 0306-2619, 2016, vol. 182, pp. 365-375
5. Boškosi, Pavle, Juričič, Dani. Inverse Gaussian mixtures models of bearing vibrations under local faults. *Mechanical systems and signal processing*, ISSN 0888-3270, 2016, vol. 66/67, pp. 546-556

### Some outstanding achievements in the past year

1. The Department of Systems and Control celebrates its 30<sup>th</sup> anniversary. On 22<sup>th</sup> of June, 2016 we celebrated this event with a barbecue and a bowling tournament (Figure 5)
2. The book entitled "Modelling and Control of Dynamic Systems Using Gaussian Process Models", authored by our Department member Prof. Dr. Juš Kocijan, has appeared in the Springer series "Advances in Industrial Control"
3. The "2016 Prešeren award" at the Faculty of Electrical Engineering, Ljubljana was awarded to our department member Tomaž Kos for his research project entitled Measurement system for automated low-frequency and high-temperature characterization of dielectric materials
4. "Jozef Stefan" Institute and the Ministry of Education, Science and Sport have signed an agreement on co-financing operation no. C3330-16-529000, "**Building Blocks, Tools and Systems for Factories of the Future**" (**GOSTOP**). Our department plays one of the main roles in this programme
5. Two new projects in the field of the development of hydrogen technologies (Memphys, Insight) were approved for financing within the scope of Horizon 2020 programme (Fuel Cells and Hydrogen Joint Undertaking)

### Awards and appointments

1. Tomaž Kos: The 2016 Prešeren award at the University of Ljubljana, Faculty of Electrical Engineering for his research project entitled Measurement system for automated low-frequency and high-temperature characterization of dielectric materials
2. Stanislav Strmčnik: received the Professor Emeritus of the University of Nova Gorica award for his significant contribution to the development of scientific activities and his remarkable performance as professor and mentor

### Patent granted

1. Janko Petrovčič, Damir Vrančič, Reducing oscillations in a control system, EP2356522 (B1), European Patent Office, 06. 01. 2016.

## INTERNATIONAL PROJECTS

1. 7FP - DIAMOND; Diagnosis-aided Control for SOFC Power System  
Prof. Dani Juričič  
European Commission
2. COST ES1202; Water\_2020: Conceiving Wastewater Treatment in 2020 - Energetic, Environmental and Economic Challenges  
Dr. Darko Vrečko  
Cost Office
3. ER-3-FU; Enabling Research; EUROFUSION  
Dr. Samo Gerškčič  
European Commission
4. Non-invasive Condition Monitoring of High Temperature Steam Electrolyser  
Prof. Dani Juričič  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Program systems and control  
Prof. Dani Juričič

## R & D GRANTS AND CONTRACTS

1. State-of-health prognostics of electrochemical energy systems  
Dr. Pavle Boškosi
2. E-maintenance of electro-mechanical drives: prognostics and health management solutions under non-stationary operating conditions  
Prof. Dani Juričič
3. Development and implementation of a method for on-line modelling and forecasting of air pollution  
Prof. Juš Kocijan
4. Optimisation of energy cost for refrigeration systems in shopping malls  
Asst. Prof. Damir Vrančič
5. Building blocks, tools and systems for the Factories of the Future - GOSTOP  
Dr. Vladimir Jovan

## NEW CONTRACTS

1. Design and assembly of diagnostic system for quality assessment of the 771 family of brushless motors  
Dr. Janko Petrovčič  
Domel, d. o. o.

2. Optimisation of energy cost for refrigeration systems in shopping malls  
Asst. Prof. Damir Vrančić  
Danfoss Trata, d. o. o.
3. Functional upgrades on existing diagnostics systems for on-line analysis of operating

characteristics and vibration measurement of motors  
Dr. Janko Petrovčič  
Domel, d. o. o.

## VISITOR FROM ABROAD

1. prof. dr. Marco Ariola, Parthenope University of Naples, Naples, Italy, 25–26 February 2016
2. prof. dr. Gianmaria de Tomassi, University of Naples Federico II, Naples, Italy, 25–26 February 2016
3. prof. dr. Alfredo Pironti, University of Naples Federico II, Naples, Italy, 25–26 February 2016
4. dr. Denis Kalupin, EUROfusion, Garching, Germany, 25–26 February 2016
5. assoc. prof. Alexandra Grancarova, University of Chemical Technology and Metallurgy, Sofia, Bulgaria, 19 May 2016
6. prof. dr. Aneta Stefanovska, Department of Physics, Lancaster University, Lancaster, United Kingdom, 6 September 2016
7. dr. Attila Gölle, University of Pannonia, Veszprém, Hungary, 12–14 October 2016
8. dr. Attila Magyar, University of Pannonia, Veszprém, Hungary, 12–14 October 2016
9. Roland Bálint, University of Pannonia, Veszprém, Hungary, 12–14 October 2016

## STAFF

### Researchers

1. Dr. Pavle Boškovski
2. Dr. Gregor Dolanc
3. Dr. Samo Gerškšič
4. Dr. Giovanni Godena
5. Dr. Dejan Gradišar
6. Dr. Nadja Hvala
7. Dr. Vladimir Jovan, Head
8. Prof. Dani Juričić
9. Prof. Juš Kocijan
10. Dr. Bojan Musizza
11. Dr. Matija Perne
12. Dr. Janko Petrovčič
13. Dr. Boštjan Pregelj
14. Prof. Stanislav Strmčnik
15. Asst. Prof. Damir Vrančić

### 16. Dr. Darko Vrečko

### Postdoctoral associates

17. Dr. Andrej Debenjak
18. Dr. Miha Glavan
19. Dr. Marko Nerat

### Postgraduates

20. Boštjan Dolenc, B. Sc.
21. Tomaž Kos, B. Sc.
22. Gjorgji Nusev, B. Sc.
23. Martin Stepančić, B. Sc.

### Technical officers

24. Stanislav Černe, B. Sc.
25. Primož Fajdiga, B. Sc.

### Technical and administrative staff

26. Maja Janežič, B. Sc.
27. Miroslav Štrubelj

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2. Pavle Boškovski, Đani Juričić, "Inverse Gaussians mixtures models of bearing vibrations under local faults", *Mech. syst. signal process.*, vol. 66/67, pp. 546-556, 2016.
3. Andraž Bradeško, Đani Juričić, Marina Santo-Zarnik, Barbara Malič, Zdravko Kutnjak, Tadej Rojac, "Coupling of the electrocaloric and electromechanical effects for solid-state refrigeration", *Appl. phys. lett.*, vol. 109, no. 14, pp. 143508-1-143508-7, 2016.
4. Nadja Damij, Pavle Boškovski, Marko Bohanec, Biljana Mileva-Boshkoska, "Ranking of business process simulation software tools with DEX/QQ hierarchical decision model", *PLoS one*, vol. 11, no. 2, pp. 0148391-1-0148391-16, 2016.
5. Gregor Dolanc, Boštjan Pregelj, Janko Petrovčič, Joachim Pasel, Günter Kolb, "Control of autothermal reforming reactor of diesel fuel", *J. power sources*, vol. 313, pp. 223-232, maj 2016.
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9. Miha Glavan, Dejan Gradišar, Damir Vrančić, "Modeliranje hladilnih elementov v nakupovalnih središčih za namene optimizacije energijskih stroškov", *Avtomatika*, vol. 2016, no. 149, pp. 42-49, 2016.
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11. Juš Kocijan, Dejan Gradišar, Marija Božnar, Boštjan Grašič, Primož Mlakar, "On-line algorithm for ground-level ozone prediction with a mobile station", *Atmos. environ. (1994)*, vol. 131, pp. 326-333, 2016.
12. Marko Nerat, Đani Juričić, "A comprehensive 3-D modeling of a single planar solid oxide fuel cell", *Int. j. hydrogen energy*, vol. 41, no. 5, pp. 3613-2627, 2016.
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2. Matjaž Bostič, Alexander Marinšek, Miha Glavan, Damir Vrančić, Iztok Humar, "Agent za upravljanje hladilnih sistemov z vidika zniževanja stroškov porabe", In: *Zbornik petindvajsete mednarodne Elektrotehniške in računalniške konference ERK 2016, 19. - 21. september 2016, Portorož*,

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Franci Gabrovšek, Martin Knez, Janja Kogovšek, Andrej Mihevc, Bojan Otoničar, Janez Mulec, Matija Perne, Metka Petrič, Tanja Pipan, Mitja Prelovšek, Tadej Slabe, Stanka Šebela, Nataša Ravbar, Nadja Zupan Hajna, "Development challenges in karst regions: sustainable land use planning in the karst of Slovenia", In: *Preserving karst environments and karst caves: karst dynamics, environments, usage and restoration: towards an international karst preservation system*, (Zeitschrift für Geomorphologie, Supplementband, N. F., vol. 60, suppl. issue 2), Elena Trofimova, ed., Jean-Nöel Salomon, ed., Stuttgart, Gebrüder Borntraeger, 2016, pp. 293-318.
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1. Martin Knez, Tadej Slabe, Franci Gabrovšek, Janja Kogovšek, Andrej Kranjc, Andrej Mihevc, Janez Mulec, Bojan Otoničar, Matija Perne, Metka Petrič, Tanja Pipan, Mitja Prelovšek, Nataša Ravbar, Stanka Šebela, Nadja Zupan Hajna, Pavel Bosák, Petr Pruner, Hong Liu, Martin Knez (urednik), Tadej Slabe (urednik), *Cave exploration in Slovenia: discovering over 350 new caves during motorway construction on classical karst*, (Cave and karst systems of the world), Cham [etc.], Springer, cop. 2016.
2. Juš Kocijan, *Modelling and control of dynamic systems using Gaussian process models*, (Advances in industrial control), Cham [etc.], Springer, cop. 2016.

## UNIVERSITY, HIGHER EDUCATION OR HIGHER VOCATIONAL EDUCATION TEXTBOOK

1. Juš Kocijan, Stanko Strmčnik, *Osnove avtomatskega vodenja*, V Novi Gorici, Založba Univerze, 2016.

## PATENT

1. Janko Petrovčič, Damir Vrančić, *Reducing oscillations in a control system*, EP2356522 (B1), European Patent Office, 06. 01. 2016.

## MENTORING

1. Giovanni Godena, *Models of batch process control software*: doctoral dissertation, Ljubljana, 2016 (mentor Stanko Strmčnik).
2. Matej Gabrijelčič, *Closed-loop control of multi-zone furnace for heat treatment of steel ropes*: master's thesis, Nova Gorica, 2016 (mentor Juš Kocijan).
3. Tomaž Kos, *Measurement system for automated low-frequency and high-temperature characterization of dielectric materials*: master's thesis, Ljubljana, 2016 (mentor Gregor Klančar; co-mentor Tadej Rojac).

# ARTIFICIAL INTELLIGENCE LABORATORY

E-3

The Artificial Intelligence Laboratory (<http://ailab.ijs.si/>) is mainly concerned with the research and development of information technologies, with an emphasis on artificial intelligence. Our main areas of research are: data analysis with an emphasis on text, web and cross-modal data, scalable real-time data analysis, machine learning, analysis and modelling of large networks, visualization of complex data, semantic technologies, language technologies, reasoning methods and knowledge management. The Artificial Intelligence Laboratory has employees and students with an international background and expertise in different areas of artificial intelligence. In addition to publishing their research results in international publications and presenting their work at international events, our researchers have also developed numerous 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 analysing 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; Qminer (<http://qminer.ijs.si/>), a data analytics platform for processing large-scale real-time streams containing structured and unstructured data; 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; EventRegistry (<http://eventregistry.org/>), a system for identifying world events in news media; Twitter Observatory (<http://twitterobservatory.net/>), a system for the analysis of selected tweets; Wikifier (<http://wikifier.org/>), a system for annotating documents with links to relevant Wikipedia pages; StreamStory (<http://streamstory.ijs.si/>), an exploratory data-stream analysis tool offering an alternative type of visualization by representing the multivariate data stream using a Markovian model; DataScienceExplorer, a dashboard for the visualizations of data science based on academic papers; Videolectures Explorer (<http://explore.videolectures.net/>), a tool enabling users to search through the lectures and find similarities between them; EDSA dashboard (<http://jobs.videolectures.net/policymakers>), a tool aggregating demand data (job postings around Europe) and supply data (training materials) in data science; nextPin (<http://traffic.ijs.si/NextPin/?user=demo>), a system for the analysis of time-varying data of geographical locations. The laboratory's strategy is to combine scientific excellence with strong industrial collaboration, enabling the transfer of research results into real-world business environments.

In the past 14 years, members of the Artificial Intelligence Laboratory have successfully completed 43 EU projects, of which 3 were concluded in 2016 and 11 were still on going. In 2016, we were also involved in 4 national projects and 1 industrial project. Together with the Department for Communication Systems (E6) in collaboration with Adria Mobil, we have continued and furthered the development of sensor technologies and artificial intelligence methods for the user-friendly and energy efficient functioning of auto-homes, which is being tested in real-world environments.

In 2016, two EU FP7 projects in the area of statistical data modelling and machine learning were successfully concluded: Symphony and FI-IMPACT. Our work in Symphony (*Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy*) focused on developing tools and approaches to support economic policy makers through analysis, prediction, and



Head:  
Prof. Dunja Mladenic

Marko Grobelnik was named Digital Champion by Slovenian government



Figure 1: Mobility patterns analytics tool showing user's mobility timeline (on right), selected place statistics (on left) and predicted next location (on map)



automated polling based on media monitoring. Our team established a social-media monitoring data infrastructure, connecting social media data with news events from our *EventRegistry* system and gathered market and macro-economic data. We implemented multi-lingual social media sentiment analysis and mainstream media geographical opinion diffusion measurements. Signals extracted from the data are fed into a scalable large-scale system of correlation analysis, together with an intuitive UI, for exposing and exploring connections between the different signals: concepts, companies, people, etc. The correlation analysis system also enables automated feature selection for the nowcasting functionality and is exposed through a friendly UI. Finally, we devised and performed experi-

ments to evaluate our methods and tools. The EU FP7 project FI-IMPACT (*Future Internet Impact Assurance*) focused on measuring and projecting the potential take-up and impact of Phase III Accelerator Projects co-funded under the Future Internet PPP, by collecting and assessing qualitative and quantitative evidence of their potential socio-economic impact to 2020. Together with the Centre for Knowledge Transfer in Information Technologies (CT3), we developed a web-based self-assessment tool to support Accelerator Projects to position their product, verify the market potential and check complementarity with other FI-PPP participants' offerings. A separate set of tools for the benchmarking of accelerator best practices has

## Organizing International conference LREC 2016

- **Introductory messages: Marko Grobelnik - Message of the Chair of the Local Organizing Committee**
- **Invited talk: Simon Krek - Slovene and the South Slavic Language Family - the Obligation of Expressing Duality and Other Stories from the South**

been developed as a set of "R" statistical tool scripts. Both the reporting environment and best-practices analysis tool have been made available as open-source projects on GitHub. In the H2020 EU project, OPTIMUM (*Multi-source Big Data Fusion Driven Pro-activity for Intelligent Mobility*), our team is building a callable big-data traffic infrastructure which serves more than 40 traffic-related APIs with the data from Slovenia and EU, both from the project consortium and public at large. Part of this data infrastructure started to be used commercially used, running inside the project partner's premises, serving their data. As part of the project, we also continue to build personal patterns detection and prediction service, which currently (experimentally) has around 3000 units sending GPS locations in real-time. This work represents the continuation of the FP7 project *Mobis*. This service is becoming the main geo-spatial analytics driver inside *OPTIMUM* as well as other analytics projects. As part of the *OPTIMUM* project and our on-going collaboration with Adria, we are also collaborating on developing custom hardware that will allow the users to control and communicate with the motor-homes, which are eventually becoming smart-connected vehicles. Within the H2020 Marie Skłodowska-Curie ITN project *BigDataFinance (Training for Big Data in Financial Research and Risk Management)* two doctoral students were recruited by our department in order

to execute two projects entitled "*Deep Knowledge Extraction from Financial, Business, and Social Text*" and "*Characterising Financial Markets from Event-driven Perspective*". In 2016, *BigDataFinance* implemented two training events. The first, entitled "Data Science in Finance", took place at the Tampere University of Technology in Finland. The second, entitled "High-Frequency Data Econometrics", took place at the Aarhus University in Denmark.

In the areas of **text and network analysis** and **language technologies**, we contributed an invited talk on "Slovene and the South Slavic Language Family - the Obligation of Expressing Duality and Other Stories from the South" at the LREC 2016 conference (Simon Krek). In 2016, together with the Department of Knowledge Technologies (E8), we continued to lead the Slovene research infrastructure CLARIN.SI, which provides easy publication and sustainable access to digital language data for scholars in the humanities and social sciences. In addition to providing support for the CLARIN.SI repository, we contributed Slovene data for the shared task on the automatic identification of verbal Multi-Word Expressions and worked on annotation of Semantic Role Label system for Slovene.

In the area of **semantic technologies**, the team's work has focused on two European projects. The EU FP7 project ProaSense (*The Proactive Sensing Enterprise*) is one of the early adapters of a shift from reactive to

proactive computing in the enterprise environment. Within the project, we have developed tools for multivariate data-stream exploration, prediction and anomaly detection. In the past year, we have successfully completed the third and last year of the EU FP7 project xLiMe (*Cross-lingual Cross-media Knowledge Extraction*), in the context of which we have been researching the real-time fusion of information extracted from multiple modalities: text, social media, audio, video and user-behaviour data. We have produced the final prototypes for semantic graph construction, opinion diffusion, behaviour analytics and speech annotation systems, and participated in the integration of our



Figure 2: The Videolectures Explorer tool showing the landscape of lectures published on Videolectures.NET and its statistics. On the left side, it shows the keywords used in the query and the basic statistics of the found lectures. On the right side, it shows the lecture landscape with landmarks.

results into a coherent project pipeline. Within the H2020 Marie Skłodowska-Curie RISE project RENOIR (*Reverse engineering of social information processing*), our work focuses on the discovery and analysis of dynamics of information publication, spreading and consumption. We conducted an extensive analysis of news bias over the global news publisher space and their coverage of millions of events. We have also developed novel methodologies for modelling causal relationships between events reported in the news and the extraction of structured information about events from news media text.

**In the area of knowledge management**, where the group's main focus includes research and development by using methods and tools from a broader Artificial Intelligence area in real business settings, we have contributed an interview in "Finance" entitled "Vodno kmetovanje: digitalizacija ribogojnic in školjčič" given by Dunja Mladenec (<http://agrobiznis.finance.si/8843345/Vodno-kmetovanje-digitalizacija-ribojnic-in-skoljicisc>) as well as an interview for RTVSlo entitled "Data modelling in aquaculture" (<http://4d.rtvsllo.si/arhiv/o-morju-in-pomors-cakih/174401690>). In collaboration with the Department for Communication Systems (E6), we have continued work on the EU FP7 project SunSeed (*Sustainable and robust networking for smart electricity distribution*). Our main task was the development and deployment of online streaming short-term load forecasting prototype. The prototype consists of two main instances: (1) Data instance and (2) Modelling instance. We have defined data interfaces for integration within the *Sunseed* analytical platform. Several data adapters were developed for connection with internal and external data sources. Streaming data aggregates were developed for each data source for the purpose of data cleaning, pre-processing and data enrichment. In the modelling instance part of the prototype, we have implemented a learning algorithm for online forecasting which is able to forecast in an online fashion. Additionally, the GUI for the prototype was developed for the purpose of testing and investing of the results. Several data visualisation tools were developed and added to the GUI for demonstration purposes. The prototype also includes REST API services for posting and requesting the latest results to the main database. Our current and future work involves scaling the prototype to be able to process and forecast the load for a larger number of nodes. Within the H2020 EU project AquaSmart (*Aquaculture Smart and Open Data Analytics as a Service*), whose aim is to lower production costs and improve the profitability and operational efficiency of fish farms, work has continued on the creation of a central framework, accessible via the web, where our tools implementing several machine-learning methods will be used to evaluate the performance of fish farms' production, identify patterns and trends, optimize feeding and growth models and estimate the fish population. In addition to analytics, we also created a translation service based on the Moses machine translation tool (5 language pairs), which will support the multi-language aspect of the project.

**Promotion of science** is continually present in the efforts of the Artificial Intelligence Laboratory. In 2016, Marko Grobelnik was named Digital Champion by the Slovenian government. Digital Champions are ambassadors for the Digital Single Market, appointed by their Member States to help every European citizen become digital. Within this role, Marko has had several interviews promoting digital technologies, one by the Slovenian press agency (<http://znanost.sta.si/2312994/novi-glasnik-digitalne-tehnologije-digitalna-tehnologija-prinasa-priloznosti-za-prijetnejse-zivljenje>), another by the national RTVSlo (<http://www.rtvsllo.si/znanost-in-tehnologija/grobelnik-novi-digitalni-glasnik-cez-5-let-se-o-uberju-verjetno-spluh-ne-bomo-vec-sprasevali/405312>). He also appeared in the weekly discussion show "Studio-City", for the topic of digitalizing Slovenia (<http://4d.rtvsllo.si/arhiv/studio-city-prispevki/174440159>). The department's success in obtaining funding from the European Commission was also reflected in 2016 in an interview given by Dunja Mladenec for "Manager" regarding how researchers obtain EU funding entitled "Spoznajte raziskovalce, ki pobirajo evropske milijone" (<http://manager.finance.si/8843441/Spoznajte-raziskovalce-ki-pobirajo-evropske-milijone?metered=yes&sid=412912399>). Within the H2020 EU project EDSA (*European Data Science Academy*), the Artificial Intelligence Laboratory contributed a dashboard aggregating demand and supply data in data science - demand data of data science job postings around Europe and supply data of data science training materials. The department participated in the EDSA curriculum development, collecting and providing materials on the curriculum topic "Statistical/Mathematical Foundations". We have developed training and learning analytics applications based on Videolectures.NET data, such as *Videolectures Explorer* (enabling users to search through the lectures and find similarities between them) and the *Videolectures Learning Analytics Dashboard* (allowing for analysis of viewer behaviour). Together with the Centre for Knowledge Transfer in Information Technologies (CT3), we continued to use the videolectures.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 2016, more than 200 students participated in the competition. We have been organizing a touring exhibition about female PhD

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**We have successfully concluded three EU FP7 projects: XLime (Cross-Lingual, Cross-Media Knowledge Extraction) (<http://xlime.eu/>), Symphony (Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy) (<http://projectsymphony.eu/>), FI-IMPACT (Future Internet Impact Assurance) (<http://www.fi-impact.net/>)**

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holders from the area of computer science in Slovenia since 2006, thereby promoting the role of women in science (<http://ScienceWithArt.ijs.si/>).

In 2016 we were very actively involved in submitting new project proposals, particularly within the H2020 Programme. Once again, we were very successful, obtaining funding for four new projects in H2020: *EwShopp*, *euBusinessGraph*, *PrEstoCloud* and *Water4Cities*. We continue with our successful efforts to include Slovenian industry into the European research area, where over the past 11 years we have produced a list of 18 companies participating in EU projects.

### Some outstanding publications in the past year

1. Karlovčec, Mario, Lužar, Borut, Mladenić, Dunja. Core-periphery dynamics in collaboration networks: the case study of Slovenia. *Scientometrics*, December 2016, Volume 109, Issue 3, pp 1561–1578
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5. Kudryavtseva, Ganna, Škraba, Primož. The principal bundles over an inverse semigroup. *Semigroup forum*, 2016, 22 pp
6. Fortuna, Carolina, De Poorter, Eli, Škraba, Primož, Moerman, Ingrid. Data driven wireless network design : a multi-level modeling approach. *Wireless personal communications*, [in press] 2016, 15 pp
7. Grobelnik, Marko, Mladenić, Dunja, Witbrock, Michael J. Text Mining For The Semantic Web. V: Sammut, Claude (ur.), WEBB, Geoffrey I. (ur.). *Encyclopedia of machine learning and data mining*. Heidelberg [etc.]: Springer, 2016, 3 pages
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9. Brank, Janez, Mladenić, Dunja, Grobelnik, Marko. Feature Construction In Text Mining. V: Sammut, Claude (Ur.), Webb, Geoffrey I. (ur.). *Encyclopedia of machine learning and data mining*. Heidelberg [etc.]: Springer, 2016, 6 pages

### Organization of Conferences, Congresses and Meetings

1. FP7 NRG4Cast, Brussels, Belgium, 25 - 26 January 2016
2. H2020 EDSA, Ljubljana, Slovenia, 8 - 10 March 2016
3. FP7 ProaSense, Ljubljana, Slovenia, 24 - 25 February 2016
4. H2020 RENOIR, Ljubljana, Slovenia, 27 - 28 June 2016

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## INTERNATIONAL PROJECTS

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| <ol style="list-style-type: none"> <li>1. ELRC - European Language Resource Coordination<br/>Dr. Simon Krek<br/>Dfki Gmbh - Deutsches Forschungszentrum Fuer</li> <li>2. Services Concerning Ethnical, Communication, Legal, Skills Issues and Methodological Cooperation related to the Use of Big Data in European Statistics<br/>Marko Grobelnik<br/>Sogeti Luxembourg S.a.</li> <li>3. 7FP - ProaSense; The Proactive Sensing Enterprise<br/>Marko Grobelnik<br/>European Commission</li> <li>4. 7FP - SYMPHONY; Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy<br/>Prof. Dunja Mladenić<br/>European Commission</li> <li>5. 7FP - xLiMe; CrossLingual CrossMedia Knowledge Extraction<br/>Marko Grobelnik<br/>European Commission</li> <li>6. 7FP - SUNSEED; Sustainable and Robust Networking for Smart Electricity Distribution<br/>Prof. Dunja Mladenić<br/>European Commission</li> <li>7. 7FP - FI-IMPACT; Future Internet Impact Assurance<br/>Marko Grobelnik<br/>European Commission</li> </ol> | <ol style="list-style-type: none"> <li>8. PARSEME: PARsing and Multi-Word Expressions. Towards Linguistic Precision and Computational Efficiency in Natural Language Processing<br/>Dr. Simon Krek<br/>Cost Office</li> <li>9. IS1305, European Network of E-Lexicography (ENeL)<br/>Dr. Simon Krek<br/>Cost Office</li> <li>10. COST CA16105; European Network for Combining Language Learning with Crowdsourcing Techniques<br/>Dr. Simon Krek<br/>Cost Office</li> <li>11. H2020 - EDSA; European Data Science Academy<br/>Marko Grobelnik<br/>European Commission</li> <li>12. H2020 - OPTIMUM; Multi-source Big Data Fusion Driven Proactivity for Intelligent Mobility<br/>Marko Grobelnik<br/>European Commission</li> <li>13. H2020 - BigDataFinance; Training for Big Data in Financial Research and Risk Management<br/>Marko Grobelnik<br/>European Commission</li> <li>14. H2020 - RENOIR; Reverse Engineering of Social Information Processing<br/>Marko Grobelnik<br/>European Commission</li> </ol> |
|--|--|

15. H2020 - MOVING; Training Towards a Society of Data-Savvy Information Professionals to enable Open Leadership Innovation  
Marko Grobelnik  
European Commission
16. H2020 - GlobalDNA; Dynamic Network of Global News Events  
Prof. Dunja Mladenić  
European Commission
17. Representation of Big Data  
Prof. Dunja Mladenić  
Slovenian Research Agency
18. Semantic Role Labeling in Slovene and Croatian  
Dr. Simon Krek  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Knowledge Technologies  
Prof. Dunja Mladenić

## R&D GRANTS AND CONTRACTS

1. Model for Domain-Specific Trend Prediction based on Semantic Enrichment of Unstructured Patterns  
Prof. Dunja Mladenić
2. Slovene scientific texts: resources and description  
Dr. Simon Krek
3. Learning Topological Representations  
Asst. Prof. Primož Škraba
4. Forbidden Books in the Slovenian Lands in the Early Modern Period  
Dr. Simon Krek

## VISITORS FROM ABROAD

1. Chris Creel, Cotiviti, Atlanta, USA, 24 February 2016
2. Janusz Holyst, Politechnika Warszawska, Warsaw, Poland, 1 - 12 March 2016
3. Janek Choloniewski, Politechnika Warszawska, Warsaw, Poland, 1 March - 8 May 2016
4. Janek Choloniewski, Politechnika Warszawska, Warsaw, Poland, 9 May - 8 July 2016
5. Dr. Jasminka Dobša, Fakultet Organizacije i Informatike, Univerza Zagreb, Varaždin, Croatia, 13 - 17 June 2016
6. Dr. Ivan Magdalenic, Fakultet Organizacije i Informatike, Univerza Zagreb, Varaždin, Croatia, 13 - 17 June 2016
7. Dr. Danijel Radošević, Fakultet Organizacije i Informatike, Univerza Zagreb, Varaždin, Croatia, 13 - 17 June 2016
8. Dr. Nicolo Cesa-Bianchi, Università degli Studi di Milano, Milano, Italy, 16 - 17 June 2016
9. Dr. Julian Sienkiewicz, Warsaw University of Technology, Warsaw, Poland, 17 June - 1 July 2016
10. Dr. Jennifer Croft, University of Iowa, Iowa City, ZUSA, 22 - 23 June 2016
11. Krzysztof Suchecki, Warsaw University of Technology, Warsaw, Poland, 22 June - 23 July 2016
12. Anna Grzywacz, Warsaw University of Technology, Warsaw, Poland, 31 August - 14 September 2016
13. Janek Choloniewski, Politechnika Warszawska, Warsaw, Poland, 9 - 10 October 2016
14. Juhana Lepasaar, Evropska Komisija, Brussels, Belgium, 25 November 2016
15. Darko Dujić, ceneje.si, Ljubljana, Slovenia, 28 November 2016
16. Matija Torlak, Big bang d.o.o., Ljubljana, Slovenia, 28 November 2016
17. Matej Žvan, cde.si, Ljubljana, Slovenia, 28 November 2016

## STAFF

### Researchers

1. Dr. Damjan Bojadžiev
2. Asst. Prof. Branko Kavšek\*
3. Dr. Simon Krek
4. Dr. Gregor Leban
5. **Prof. Dunja Mladenić, Head**
6. John Stewart Shawe-Taylor, B. Sc.
7. Asst. Prof. Primož Škraba

### Postdoctoral associates

8. Dr. Janez Brank
9. Dr. Mario Karlovčec
10. Dr. Aljaž Košmerlj
11. Dr. Jurij Leskovec
12. *Dr. Andrej Muhič\**, left 01.10.16
13. Dr. Inna Novalija
14. *Dr. Joao Paulo Pita Da Costa\**, left 01.09.16
15. Dr. Jan Rupnik
16. Dr. Polona Škraba Stanič

17. Luka Bradeško, B. Sc.
18. Dr. Blaž Fortuna
19. Rayid Ghani, M. Sc.
20. *Dejan Govc\**, left 01.10.16

21. James Alexander Hodson, B. Sc.

22. Mitja Jermol, M. Sc.
23. Blaž Kažič, B. Sc.
24. Klemen Kenda, B. Sc.
25. Blaž Novak, B. Sc.
26. *Janez Starc, B. Sc., left 01.06.16*
27. Luka Stopar, B. Sc.
28. Miha Torkar, B. Sc.

### Technical officers

29. Flavio Fuart, B. Sc.
30. *Darja Grošelj, B. Sc., left 23.11.16*
31. Zala Herga, B. Sc.
32. *Dr. Ganna Kudryavtseva\**, left 01.10.16
33. Matjaž Rihtar, B. Sc.
34. Maja Škrjanc\*, B. Sc.

### Technical and administrative staff

35. Aleš Buh
36. Marko Grobelnik
37. Mojca Kregar Zavrl, B. Sc.
38. Mateja Škraba, B. Sc.

Note:

\* part-time JSI member

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Austin R. Benson, David F. Gleich, Jurij Leskovec, "Higher-order organization of complex networks", *Science (Wash. D.C.)*, vol. 363, no. 6295, pp. 163-166, 2016.
2. Carolina Fortuna, Eli De Poorter, Primož Škraba, Ingrid Moerman, "Data driven wireless network design: a multi-level modeling approach", *Wirel. pers. commun.*, vol. 88, no.1, pp. 63-77, 2016.
3. Polona Gantar, Iztok Kosem, Simon Krek, "Discovering automated lexicography", *International journal of lexicography*, vol. 29, issue 2, pp. 200-225, 2016.
4. Dejan Govc, "On the definition of the homological critical value", *J. homotopy relat. struct.*, vol. 11, iss. 1, pp. 143-151, 2016.
5. Mario Karlovčec, Borut Lužar, Dunja Mladenić, "Core-periphery dynamics in collaboration networks: the case study of Slovenia", *Scientometrics*, vol. 109, iss. 3, pp. 1561-1578, 2016.
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7. Ganna Kudryavtseva, Primož Škraba, "The principal bundles over an inverse semigroup", *Semigroup forum*, 22 pp., 2016.
8. João Pita Costa, Karin Cvetko-Vah, "Flat coset decompositions of skew lattices", *Semigroup forum*, vol. 92, no. 2, pp. 361-376, 2016.
9. Georg Rehm *et al.* (44 authors), "The strategic impact of META-NET on the regional, national and international level", *Language resources and evaluation*, vol. 50, no. 2, pp. 351-374, 2016.

10. Jan Rupnik, Andrej Muhič, Gregor Leban, Primož Škraba, Blaž Fortuna, Marko Grobelnik, "News across languages - cross-lingual document similarity and event tracking", *J. artif. intell. res.*, vol. 55, pp. 283-316, 2016.
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12. Nenad Tomašev, Krisztian Buza, Dunja Mladenič, "Correcting the hub occurrence prediction bias in many dimensions", *Comput. Sci. Inf. Syst.*, vol. 13, no. 1, pp. 1-21, 2016.

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1. Špela Arhar Holdt, Darja Fišer, Tomaž Erjavec, Simon Krek, "Syntactic annotation of Slovene CMC: first steps", In: *Proceedings of the 4th Conference on CMC and Social Media Corpora for the Humanities, 27-28 September 2016, Faculty of Arts, University of Ljubljana, Ljubljana, Slovenia*, pp. 3-6.
2. Katja Berčič, Gabriella Cattaneo, Mario Karlovčec, Flavio Fuat, Gaber Cerle, "Application of advanced analytical techniques in support of socio-economic impact assessment of innovation funding programmes", In: *Izkopavanje znanja in podatkovna skladišča (SiKDD): zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10. oktober 2016, [Ljubljana, Slovenija]: zvezek D*, pp. 9-12.
3. Jan Chotoniowski, Gregor Leban, Sebastijan Maček, Aljoša Rehar, "Information flow between news articles: Slovene media case study", In: *Izkopavanje znanja in podatkovna skladišča (SiKDD): zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10. oktober 2016, [Ljubljana, Slovenija]: zvezek D*, pp. 13-16.
4. Ruben Costa, Ricardo Jardim-Gonçalves, Paulo Figueiras, Margherita Forcolin, Mitja Jermol, Richards Stevens, "Smart cargo for multimodal freight transport: when "cloud" becomes "fog"", In: *8th IFAC Conference on Manufacturing Modelling, Management and Control MIM 2016, Troyes, France, 28-30 June 2016, IFAC-PapersOnline*, vol. 49, no. 12, pp. 121-126, 2016.
5. Zala Herga, Jan Rupnik, Primož Škraba, Blaž Fortuna, "Modeling probability of default and credit limits: Slovene media case study", In: *Izkopavanje znanja in podatkovna skladišča (SiKDD): zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10. oktober 2016, [Ljubljana, Slovenija]: zvezek D*, pp. 21-24.
6. Matic Kladnik, Blaž Fortuna, Pat Moore, "Big data analysis combining website visit logs with user segments and website content", In: *Izkopavanje znanja in podatkovna skladišča (SiKDD): zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10. oktober 2016, [Ljubljana, Slovenija]: zvezek D*, pp. 25-28.
7. Simon Krek, Polona Gantar, Kaja Dobrovoljč, Iza Škrjanec, "Označevanje udeleženskih vlog v učnem korpusu za slovenščino", In: *Zbornik konference Jezikovne tehnologije in digitalna humanistika, 29. september - 1. oktober 2016, Filozofska fakulteta, Univerza v Ljubljani, Ljubljana, Slovenija*, pp. 106-110.
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## MENTORING

1. Jan Rupnik, *Multi-view canonical correlation analysis*: doctoral dissertation, Ljubljana, 2016 (mentor Dunja Mladenič; co-mentor John Shawe-Taylor).
2. Andreas Thalhammer, *Linked Data Entity Summarization*: doctoral dissertation, Karlsruhe, 2016 (mentor Rudi Studer; co-mentor Dunja Mladenič).
3. Erik Novak, *Nenegativna matrična faktorizacija*: master's thesis, Ljubljana, 2016 (mentor Bor Plestenjak; co-mentor Andrej Muhič).
4. Blaž Sovdat, *Text mining via homology*: master's thesis, Ljubljana, 2016 (mentor Primož Škraba; co-mentor Sergio Cabello).

# 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, as well as information-society services and applications, especially those that ensure an efficient and pervasive life-long learning concept.***

In 2016, 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 Horizon 2020 project “Flex4Grid”, 7FP projects “COURAGE”, “EmployID” and “REDIRNET”, the “eSENS” project from the CIP (Competitiveness and innovation) programme, the “SENDER” project from the ISFP programme, the EU DG Justice “LIVE\_FOR” project, the “GIRDA” project from the Erasmus+ programme, and the national basic research project. 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 2016 they were the mentors of two finished PhD theses, four Master theses, and two diploma theses.



Head:

**Prof. Borka Jerman Blažič**

### Concepts and architectures of the secure future internet

The first area of R&D 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 a large-scale eSENS pilot from the EU Competitiveness and innovation (CIP) programme.

The “Electronic Simple European Networked Services (eSENS)” project is consolidating the building blocks of several large-scale pilots, e.g., 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 the project activities on trust-model implementation in the piloting domains, such as e-procurement, e-health, e-justice, and business lifecycle. The aim is to elaborate (through cooperation with implementation and testing experts) the current trust models in each of the pilots concerned with the project, analyse their completeness with respect to a pre-designed framework, and extract recommendations for further development based on that framework. Furthermore, the laboratory is included in the assessment of the cyber-security principles integrated into the European interoperability reference architecture (EIRA) developed by the project.

In 2016 we have successfully finished 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 has been performed within the frame of the EU FP7 “Emergency Responder Data Interoperability Network (REDIRNET)” project. Our main activities in 2016 included ontology specification and security and a usability evaluation of the developed system. We prepared security recommendations and guidelines for the developers and users of the REDIRNET system. Good practices and modern security challenges faced by the public safety agencies were taken into account. A combination of analytical and empirical evaluation methods (U2XEM) was employed to assess the system’s usability and user experience. The final demonstration and practical evaluation of the REDIRNET system with users took place in June 2016 in Bratislava, Slovakia. We presented security aspects of the public safety data interoperability network at an international conference in Sweden, and the specified ontology at a conference in Spain.

In 2016 we continued with the “Prosumer Flexibility Services for Smart Grid management (Flex4Grid)” project from the Horizon 2020 EU programme. The project is part of the call for Competitive low-carbon energy from the Societal Challenges pillar. Based on innovative use of ICT technologies the project aims at improving the smart-grid operation by utilizing the prosumers flexibility. The project has a strong Slovenian contribution with Elektro Celje and Smart Com as partners in the project, besides the Jožef Stefan Institute. Slovenian partners are working together to realize a large-scale pilot in the Celje region. So far, we have developed basic elements and services that enable

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**We have created building blocks for security infrastructures and trusted services.**

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prosumers flexibility management, from home gateways to smart mobile applications. The laboratory focus was on cloud storage and processing services, data analytics with forecasting, and security and privacy provisioning. At the end of 2016 a test pilot evaluation of the project system started in Slovenia. Currently, 100 users are involved, while in 2017, a long-term pilot is planned with 2500 users.

The Laboratory for Open Systems and Networks is also involved in a 3-year national project EkoSmart (Ecosystem of a smart city) with the main focus on health, mobility, active lifestyle and well being. The project started in August 2016 and has six research programs to help build an ecosystem for safer and better quality living for individuals and communities alike, based on innovative IKT solutions. The Laboratory for Open Systems and Networks takes part in the Electronic Mobile Health research program, where operative directions include information technologies for whole health care, home support, mobile monitoring of vital and environmental data, method and algorithms development, and the development of corresponding IKT platforms. Our main role within the project is the development of methods and algorithms for personal health data anonymization. Models, such as k-anonymity, l-diversity, and LKC-privacy, will be considered for the protection of personal data privacy. Among other R&D challenges we will also focus on algorithms and mechanisms for the safety of collected data (access and storage), as well as designing machine-learning applications for disease discovery in databases and intelligent support for treatment monitoring.

Under the Infrastructure program in research organizations we again 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.

### Security and privacy in information systems

The provision of security and privacy services is crucial for the modern information society. In 2016 our R&D activities in this field were focused on the fight against cybercrime, novel security mechanisms, such as graphical authentication, and trust systems. The results have been published in a scientific book, seven journal papers, and several conference papers at international conferences.

The main goal of the “Cybercrime and cyberterrorism European research agenda (COURAGE)” project was the definition of the R&D agenda in the area of the fight against cybercrime and cyberterrorism (CC/CT). Cybercrime is described as behaviour in which computers or networks are a tool, a target, or a place of criminal activity. The agenda that was finalized in 2016 identifies the major challenges, reveals research gaps, and identifies and recommends detailed practical research approaches to address those gaps through strategies that are aligned to the real-world needs. In total, 12 items that need further research are described by the agenda, for example, definition, characteristics and behaviour of the offenders and victims in cybercrime events, advanced tools for digital investigation in compliance with privacy legislation and regulation, preventing and countering CC/CT activities on the dark web and similar networks, and definition and harmonisation of CC/CT terminology throughout the EU. The agenda recommends short-, mid- and longer-term actions for each of the described research items and the roles of different stakeholders (law-enforcement agencies, solution providers, research and technology organisations, policy makers, legal, ethical and societal stakeholders, accreditation and certification bodies, and educational institutions) in the actions. The main results were also published by Springer in a book with a title “Combating Cybercrime and Cyberterrorism: Challenges, Trends and Priorities” where we contributed a chapter “Towards the Development of a Research Agenda for Cybercrime and Cyberterrorism - Identifying the Technical Challenges and Missing Solutions”, and presented at an international conference.

### We co-design the R&D agenda in the area of the fight against cybercrime.

The fight against cybercrime is also the main goal of the SENTER (Strengthening European Network Centres of Excellence in Cybercrime) project that started in 2016. SENTER aims at creating a single point of reference for EU national cybercrime centres of excellence (CoE) and developing further the network of national CoE into a well-defined and well-functioning community. The Laboratory for Open Systems and Networks is one of the ten CoEs in cybercrime that are involved in the project. Our main activities in 2016 included preparation of an inventory of best practice material (educational resources, IT tools, expertise) in the area of the fight against cybercrime, as well as preparation of guidelines on the establishment and management of cybercrime centres of excellence. The research activities were also carried out within the two special interest groups formed by the project, i.e., OSINT (Open source intelligence) and Digital forensics.



Figure 1: The LIVE\_FOR project

Challenges, Trends and Priorities” where we contributed a chapter “Towards the Development of a Research Agenda for Cybercrime and Cyberterrorism - Identifying the Technical Challenges and Missing Solutions”, and presented at an international conference.

The fight against cybercrime is also the main goal of the SENTER (Strengthening European Network Centres of Excellence in Cybercrime) project that started in 2016. SENTER aims at creating a single point of reference for EU national cybercrime centres of excellence (CoE) and developing further the network of national CoE into a well-defined and well-functioning community. The Laboratory for Open Systems and Networks is one of the ten CoEs in cybercrime that are involved in the project. Our main activities in 2016 included preparation of an inventory of best practice material (educational resources, IT tools, expertise) in the area of the fight against cybercrime, as well as preparation of guidelines on the establishment and management of cybercrime centres of excellence. The research activities were also carried out within the two special interest groups formed by the project, i.e., OSINT (Open source intelligence) and Digital forensics.

Laboratory for Open Systems and Networks is coordinating the LIVE\_FOR (Criminal Justice Access to Digital Evidences in the Cloud - LIVE\_FORensics) project from the EU DG Justice programme. Our partners in this 2-year project that was launched in November 2016 are universities from Belgium (Vrije Universiteit Brussel), Spain (Polytechnic University of Catalonia and Autonomous University of Madrid), Germany (Fachhochschule Albstadt - Sigmaringen), and Czech Republic (Masaryk University). The LIVE\_FOR project is one of the vehicles that will bring knowledge and understanding of the new modern technologies being developed for carrying out digital investigation in the cloud-computing environment. In addition, the LIVE-FOR project will investigate the current status of the Directive 2014/41/EU implementation in the EU members' legislation, raise the awareness of the prosecutors and investigators of the new European tool for collecting cross-border evidences in the connected digital world, establish a collection of best practices, and develop standard educational content for training and education in the area of digital forensics. The project will upgrade the competence of judicial authorities in the field of cloud forensics and the use of a European investigation order in criminal matters through several activities that include joint meetings, educational and training workshops, setting up of information centres, and provision of strong awareness and dissemination activities. The project team is also committed to set up cooperation and people networking among all stakeholders in the area of the fight against cybercrime and cyberterrorism, especially prosecutors, judges, law-enforcement agencies, investigators, civil entities working in the prevention of cybercrime and cyberterrorism, business entities, and higher-educational institutions with programs in information security, fight against cybercrime, and digital forensics.

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**Our R&D results lead to a more secure information society.**

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Trust management plays an important role in security, dependability, and privacy provision. We have shown trust systems to be lacking some crucial systemic features, which helped define a novel systemic taxonomy of trust. Through an empirical study, the consideration of the human factor was shown to be a major reason for the unpredictable behaviour of trust systems. Recommendations based on Choice architecture were given for an improvement of their design. A formal model for designing trust systems with a limited amount of user bias was also proposed and tested on a static dataset. In the end, a step-by-step design procedure was defined for designing user-centric and context-dependent trust systems. The results were published in a journal "Behaviour & Information Technology" with a high citation impact factor.

Secure authentication is still an issue in the provision of trusted internet services. The problems are connected with safety and security, but at the same time with ease of use and user adoption of the application. Numerous graphical authentication approaches have been proposed on how to address the security and usability, and provide friendlier, but secure authentication. However, the user approach towards graphical password selection and the inherent personal bias in selecting images are still unclear. In 2016 we had a study published in an SCI journal where we investigated user choices in password selection for graphical-based systems for authentication. The study was based on a group of 302 participants that had been using a graphical authentication system during a period of 6 weeks. The results obtained have shown preferences for some image properties like colour, shape, and category. The study provides recommendations for service providers of graphical authentic systems for system design and for the set of graphical choices offered to the users.

In the field of privacy protection in mobile networks and mobile devices we had another study of the data privacy and personal security risks incurred by mobile users published. Our newest results appeared in the "Telematics and informatics" and "Information development" journals.

### Technology-enhanced learning

The main focus of the R&D activities in the area of technology-enhanced learning was on serious games and new e-learning services and platforms for public employment services.

The main goal of the "Scalable cost-effective facilitation of professional identity transformation in public employment services (EmployID)" project 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 privacy principles, and are compliant with the newest EU privacy and data-protection legislation. Among other main results of our R&D activities in 2016 we need to mention visualisation of learner's personal development, and the development and



Figure 2: 25 years since the first internet connection in Slovenia



evaluation of a community of practice platform for public employment services. The results have been published in a book with the title “Empowering change in public employment services – The EmployID approach”.

The overall goal of the “Gameplay for Inspiring Digital Adoption (GIRDA)” project that started in 2016 is to address the problem of the digital divide, and barriers to learning and adoption faced by older citizens who often have no digital skills. Seven partners from Slovenia, UK, Austria, and Macedonia will investigate the efficacy of an alternative approach to facilitating digital literacy and digital adoption based on digital games designed for adults. Digital learning environments, such as touch-table games, will be used to introduce individuals to digital interaction. The project will develop and deliver new and innovative education materials and methods for learners, as well as best-practice guides for those involved in promoting digital literacy.

#### Promotion of Science

In October 2016 we celebrated the 25<sup>th</sup> anniversary of the first international internet connection in Slovenia that was established in 1991 in the Laboratory for Open Systems and Networks. The connection was a result of the EUREKA-8/COSINE (Cooperation of Open Systems Interconnections) project, where the laboratory was involved. The programme of the celebration event was dedicated to young people who presented their view on the meaning of the internet for everyday life, benefits and drawbacks, as well as opinions on the future of the internet. The main invited speaker was European Commissioner Violeta Bulc, while the head of laboratory, prof. dr. Borka Jerman-Blažič, explained what was going on in 1991 when the internet connection was being set up, and gave an overview of the current R&D activities of the EU Horizon 2020 programme and the internet of the future.

#### Some outstanding publications in the past three years

1. Callanan, Cormac, Jerman-Blažič, Borka, Jerman Blažič, Andrej. User awareness and tolerance of privacy abuse on mobile internet: an exploratory study. *Telematics and informatics*, ISSN 0736-5853, 2016, vol. 33, iss. 1, pp. 109-128.
2. Pavleska, Tanja, Jerman-Blažič, Borka. User bias in online trust systems: aligning the system designers' intentions with the users' expectations. *Behaviour & information technology*, ISSN 0144-929X. [Print ed.], [in press] 2016, 15 pages.
3. Mihajlov, Martin, Jerman-Blažič, Borka, Ciunova Shuleska, Anita. Why that picture? Discovering password properties in recognition-based graphical authentication. *International journal of human-computer interaction*, ISSN 1044-7318, 2016, vol. 12, iss. 12, pp. 975-988.

#### Organization of conferences, congresses and meetings

1. Organization of the “25<sup>th</sup> Anniversary of the first Internet connection in Slovenia”, Ljubljana, October 10 2016
2. Organisation of the LIVE\_FOR project (“Criminal Justice Access to Digital Evidences in the Cloud – LIVE\_FORensics”) Kick-off meeting, Ljubljana, November 15 2016

#### Awards and Appointments

1. Primož Cigoj: The Second best Innovation: “MUPOSS” product, 9th International Technology Transfer Conference, Brdo pri Kranju, Slovenia, September 21 2016

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## INTERNATIONAL PROJECTS

1. 7FP - EmployID; Scalable Cost-effective Facilitation of Professional Identity Transformation in Public Employment Services  
Asst. Prof. Tomaž Klobučar  
European Commission
2. 7FP - REDIRNET; Emergency Responder Data Interoperability Network  
Prof. Borka Džonova Jerman Blažič  
European Commission
- 7FP - COURAGE; Cybercrime and cyberterrorisim (E)Uropean Research AGenda  
Prof. Borka Džonova Jerman Blažič  
European Commission
3. CIP-e-SENS; Electronic Simple European Networked Services  
Prof. Borka Džonova Jerman Blažič  
European Commission
4. D-FET; Dynamic Forensics Evaluation and Training  
Prof. Borka Džonova Jerman Blažič  
European Commission
5. SENTER - Strengthening European Network Centres of Excellence in Cybercrime

- Prof. Borka Džonova Jerman Blažič  
European Commission
6. ERASMUS+; GIRDA - Gameplay for Inspiring Digital Adoption  
Prof. Borka Džonova Jerman Blažič  
European Commission
7. LIVE\_FOR; Criminal Justice Access to Digital Evidences in the Cloud - LIVE\_FORensics  
Prof. Borka Džonova Jerman Blažič  
European Commission
8. H2020 - Flex4Grid; Prosumer Flexibility Services for Smart Grid Management  
Dr. Dušan Gabrijelčič  
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. Smart City Ecosystem - EkoSmart  
Dr. Živa Stepančič

## NEW CONTRACTS

1. Guidelines for the integration of service providers with SI-PASS  
Asst. Prof. Tomaž Klobučar  
Ministry of Public Administration of the RS

## STAFF

### Researchers

1. Asst. Prof. Tanja Arh\*
2. Asst. Prof. Rok Bojanc\*
3. Prof. Borka Džonova Jerman Blažič, Head
4. Dr. Dušan Gabrijelčič
5. Asst. Prof. Tomaž Klobučar

### Postdoctoral associates

6. Dr. Matej Babič
7. Dr. Tanja Pavleska
8. Dr. Živa Stepančič

### Postgraduates

9. Primož Cigoj, B. Sc.
  10. Blaž Ivanc, B. Sc.
  11. Andrej Jerman Blažič, M. Sc.
- Technical officers
12. David Djurič, B. Sc.
- Technical and administrative staff
13. Tatjana Martun, B. Sc.

### Note:

\* part-time JSI member

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### ORIGINAL ARTICLE

1. Matej Babič, "A new hybrid - system method of Machine Learning using a new method of fractal geometry and a new method of graph theory", *Elektrotehniški vestnik*, vol. 83, no. 1/2, pp. 42-46, 2016.
2. Matej Babič, "New hybrid system using in modelling process of hardening with intelligent system", *Acta Mech. Slovaca (Košice)*, vol. 20, no. 1, pp. 34-40, 2016.
3. Matej Babič, "New method for determination of microstructure of heat treatment materials", *Journal of production engineering*, vol. 19, no. 1, pp. 91-94, 2016.
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4. Blaž Ivanc, Borka Jerman-Blažič, "Development approach to the attack modeling for the needs of cyber security education", In: *Proceedings, The Third International Conference on Digital Information Processing, Data Mining, and Wireless Communications, DIPDMWC2016, July 06-08 2016, Moscow, Russia*, pp. 216-220.
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### PUBLISHED CONFERENCE CONTRIBUTION

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1. Borka Jerman-Blažič, Tomaž Klobučar, "Towards the development of a research agenda for cybercrime and cyberterrorism - identifying the technical challenges and missing solutions", In: *Combatting cybercrime and cyberterrorism: challenges, trends and priorities*, (Advanced sciences and technologies for security applications), Babak Akghbar, ed., Ben Brewster, ed., [S. l.], Springer, 2016, pp. 157-174.

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1. Graham Attwell *et al.* (27 authors), *Empowering change in public employment services: the EmployID approach*, [S. l.], European Union's, 2016.

## PROFESSIONAL MONOGRAPH

1. Borka Jerman-Blažič, Cormac Callanan, *User tolerance for privacy abuse on mobile Internet*, Saarbrücken, LAP Lambert, 2016.

## MENTORING

1. Tanja Pavleska, *Alleviating user bias in online trust systems*: doctoral dissertation, Ljubljana, 2016 (mentor Borka Jerman Blažič).

2. Mateja Gorenc, *Abuse of internet services in the workplace and the emergence of addiction*: doctoral dissertation, Celje, 2016 (mentor Borka Jerman Blažič; co-mentor Anita Goltnik Urnaut).
3. Neda Bogdanović Golić, *E-support for the project management*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič).
4. Matija Jekovec, *Improving the customer service support for on-line users by introducing modern web technologies*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič).
5. Aleš Leskošek, *Software asset management as a service*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič; co-mentor Tomaž Turk).
6. Tanja Marolt, *The security of electronic banking: an analysis of the situation in Slovenia*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič).
7. Dušan Rehberger, *Renewing of the informational infrastructure with the IPV6 technology in the Slovenian environmental agency*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič).
8. Luka Škof, *An analysis of cyber-crime and its economic damage assessment*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič).
9. Goran Uršič, *Introducing modern telecommunication technologies and services in electro-distribution companies: the case of a transmission system operator*: master's thesis, Ljubljana, 2016 (mentor Borka Jerman Blažič).
10. Matevž Mahorčič, *Introduction of the B2B ICT-service at Vomit d. o. o.*: master's thesis, Maribor, 2016 (mentor Tanja Arh).
11. Franci Rojc, *Feasibility study of the introduction of a document system in SAP at Kolektor Group d. o. o.*: master's thesis, Maribor, 2016 (mentor Tanja Arh).

# 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 three laboratories, 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 2016 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 research program on Communication networks and services (P2-0016) the emphasis was on research in the areas of: radio propagation, access architectures for heterogeneous wireless networks, management of radio and network resources and cognitive communications.

The investigation of the radio-signal propagation was focused on two main topics. The first topic concerns the research on radio-signal propagation in special environments, such as caves, long road and railway tunnels. The emphasis was on radio-wave propagation characteristics in curved tunnels for designing reliable communications in subway tunnels. The extensive propagation measurements conducted in subway tunnels provide an insight into the large-scale fading characteristics in real curved subway tunnels at various frequencies (920 MHz, 2400 MHz, in 5705 MHz). The qualitative analysis and corresponding findings are useful for realizing the intelligent transportation system in subway and railway systems as well the provision of wireless communications in caves in the case of emergency.

The second topic concerns the development, implementation and testing of a software tool for radio-wave propagation modelling in mobile communication systems and the optimization of wireless communication systems. The tool is integrated into an open-source geographical information system (GIS) and incorporates statistical models, channel models based on ray tracing and optimization procedures. We studied computationally efficient radio ray-tracing techniques in the context of physical channel models.

In 2016 we started an applied project in collaboration with Xlab and Alanta on advanced ray-tracing techniques in radio environment characterization and radio localization. The project builds upon our research efforts from the past years on adapting algorithmic concepts known from ray tracing in computer graphics to radio environment modelling, where we have already proposed the efficient use of the massively parallel hardware of graphical processors. Our approach to divergence handling in the single instruction multiple thread (SIMT) architectures is applicable to a wider set of problems that can be solved on graphical processors.

We applied the concept of rasterization-like discretization to the classic method of images, which is a well-established method of deterministic radio-propagation modelling. Instead of a computational geometry approach, the spatial coherence of the electromagnetic propagation of surface-reflected or refracted rays is treated simultaneously in rendering-like steps. The proposed rasterization is of a comparable run time to that of the fundamentally parallel shooting and bouncing rays while retaining the superior computational accuracy.

Furthermore, we focused on wireless network optimization using a multi-objective evolutionary algorithm, which determines for a given set of criteria functions the optimal network parameters. The aim of the proposed solution is to maximize the network efficiency, reduce the needed resources and consequently reduce the opera-



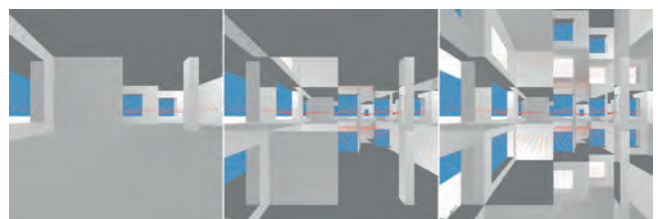
Head:

**Prof. Mihael Mohorčič**

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**We applied the concept of rasterization-like discretization to the classic method of images, and thus relaxed the computing requirements with respect to the intensive computational geometry procedures.**

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*Figure 1: Radio-signal reflections and refractions are recursively traversed using graphic primitives. The illustration shows three snapshots of a framebuffer object at increasing tree depth with black-and-white rendering of the scene objects and visible reception points superimposed as red dots.*

tional costs. Based on the terrain profile maps and construction locations, the tool calculates the path loss by applying state-of-the-art statistical models and determines the optimal base-station locations and their parameters by maximizing defined criteria functions. The implemented solution is generic and it could be used for planning any heterogeneous wireless network by appropriately adjusted criteria functions. The optimization algorithms have been included in the GRASS RaPlAT framework and applied for the optimization of frequency channel allocation in the digital wireless system for the Public protection and relief forces of the Republic of Slovenia that is operating in the VHF frequency band.

In collaboration with European partners within the H2020 project eWine “elastic WiREless Networking Experimentation” we started the investigation of the wireless elastic networks that can scale to the needs of users and services through the use of intelligent software and flexible hardware. Within the project, the Communication Technology Laboratory is focused on problems related to retrieving and processing the location of a user as a context of communications applicable for the optimization of wireless communication systems. In an outdoor environment we succeeded to bring the location error close to 1 metre by using radio environment properties and measured received signal level. In the indoor environment we increased the localization precision by using an ultra-wide band (UWB) radio signal by not considering non-line-of-sight connections in triangulation of the user.

**In collaboration with the company ComSensus we developed two wide area measurement system (WAMS) devices for the use in smart grids: a synchro-phasor measurement (CP-SPM) device and a power quality measurement and control (PMC) device.**

We continued the investigation of advanced concepts and technologies for a capacity increase of wireless mesh networks using network-coding techniques, focusing on the development of advanced adaptive network coding algorithms and their adapted routing procedures. In addition, the design aspects for network-coding-enabled wireless mesh networks and applications were investigated and analysed. We showed that opportunistic network coding can improve the performance of different networks and supported applications in terms of throughput, delay and jitter; however, these benefits are more prominent if the usage of opportunistic network coding is considered upfront in the wireless-network design phase.

In 2016 we successfully concluded the SatProSi-Alpha project, carried out for the European Space Agency (ESA). The purpose of the project was to investigate the atmosphere impacts on radio-wave propagation. Up to now, these effects were rather unexplored, especially at Q-band (39.4 GHz). The experience and measurement results obtained in the project with a newly developed 4-channel Alphasat beacon receiver on the rooftop of JSI will enable engineers to develop an efficient communication technology at high-frequency bands and hence enable high satellite communication throughputs of the order of terabits/s. The measurement results were analysed in collaboration with and contributed to the international European group ASAPE (Group of the AlphaSat Aldo Paraboni propagation Experimenters).

In 2016 we started with active participation in the COST Action 15104 IRACON “Inclusive radio communication networks for 5G and beyond”, where we are contributing to several disciplinary working groups, mainly DWG-1 radio channel, DWG-2 physical layer and DWG-3 network layer, as well in some experimental working groups: EWG-LT localization and tracking and EWG-IoT Internet of things.

In the scope of the FP7 SUNSEED project “Sustainable and robust networking for smart electricity distribution”, which aims at the efficient use of the communications infrastructure in smart grids, we applied our research expertise in the field of optimization and management of communication networks also to the field of smart grids. In the last period we were focused on the development of software modules and algorithms for a three-phase estimator in the distribution network. We investigated the optimal placement of synchronized phasor measurement units in the distribution network for the most efficient state estimation and developed software modules for the analysis and visualisation of the state of the distribution network. We also implemented an algorithm for the synchronized phasor measurement unit and optimised it for running in a low-cost device with restricted capabilities.

In the **Parallel and Distributed Systems Laboratory**, we successfully continued interdisciplinary research work in the framework of the research program 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. We also cooperate with researchers from industry and medicine on research projects and with joint papers.



Figure 2: Distribution network state (Kromberk).

The basic tasks of our laboratory are the investigation of computer algorithms efficiently implementable on parallel and distributed computers and their testing on a 152-core research computer cluster with a flexible inter-connection network. The cluster is a part of a cloud established in cooperation with our research and industrial partners. We continued investigations in the field of massive data flows in body sensor networks, flows that exceed the performances of personal computers and require HPC computing and communication resources.

We successfully started to work on a FWO project “Multi-analysis of fretting fatigue using physical and virtual experiments”, which resulted in a journal article and several conference articles. In the project consortium we cooperate with researchers from the University of Ghent and the University of Luxembourg. Our task is to design and implement parallel programmes, making possible the accurate simulation of fretting-cracks propagation.

Within an R&D project obtained in a public call from the industrial partner ELES, we together with research partners from the Milan Vidmar Institute and the Slovenian Environment Agency developed and validated a DTRi (Dynamic Thermal Rating - icing) model, on the basis of which we implemented a prototype system for the operative forecasting and prevention of icing on high-voltage power transmission lines. We have validated the prototype system with measurements on an experimental site and through the reconstruction of two real cases from 1.2.2014 and 5.1.2016 on the Beričevo-Divača line. Based on promising results, the contractee decided to put the DTRi system also into the SUMO (System for the Assessment of Operating Limits) operative environment, for which we obtained additional funding from the FP7 TETRACOM project.

We continued the transfer of knowledge related to a wearable ECG measuring device and the associated software for ECG visualisation and analysis. The innovation in the extent of 5 FTE has been bought by an industrial partner, with whom we have also signed contracts for the maintenance and further development of the software and hardware. The ECG measuring device is small and unobtrusive when worn, transmits long-term (weekly, monthly and longer) measurements wirelessly to a smartphone or tablet, and is able to work on battery power for a few days. Devices like this one will represent the base of future tele-health services, which are indispensable for lowering the cost of the general health services. Our ECG wearable device was also certified as a medical device, with which we successfully concluded an FP7 TETRACOM project.

The EkoSmart (Smart City Ecosystem) proposal to the national project call “RRI in chains and value networks” of the Ministry of Education, Science and Sport was accepted. We have already started to work on the project, most notably on implementing the pilot studies about using a wearable ECG measuring device in the medical environment, and on the research of the options for analysing and integrating the measured long-term data into the existing medical records.

A project “Graph optimization and big data” was chosen for financing in the bilateral project call by the Slovenian and Hungarian research agencies. The project addresses the Big Data challenge interpreted in terms of graph models and their processing. Its goals are the proving of theorems about model parameters (chromatic number, independence number, etc.), the design of efficient parallel algorithms for model analysis and the implementation of those algorithms on supercomputers of the next generation (exascale computing). The investigations will contribute results important for graph theory (and discrete mathematics in general) and algorithms, and procedures directly applicable for the more efficient processing of Big Data. The work has already started and the first joint conference article has been published.

In the field of formal methods for discrete event systems, we developed two methods for the synthesis of more efficient conformance tests for final state machines. Besides this we continued our research of the E-LOTOS language for the specification of concurrent real-time reactive systems and proposed operators for the finer specification of reversibility.

In the **Networked Embedded Systems Laboratory** we continued in 2016 the research and development in the fields of the Internet of Things and cognitive communications. The emphasis was placed on the vertical integration of different wireless sensor and communication network technologies in support of the development and introduction of new applications. As the core building block we were using and upgrading the modular platform VESNA, used for the development of wireless sensor networks. We developed a set of new hardware modules and the corresponding software for UWB communication, for the communication with spread spectrum LoRa, for advanced signal processing using onboard DSP chip and for the support of the Linux operating system. A variety of supported features, protocols and technologies, together with an arbitrary combination of developed hardware



Figure 3: The majority of the innovation team at the presentation of the wearable ECG measuring device

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**With public-private financial investment we have completed the transfer of knowledge about a wearable ECG measuring device to the industry.**

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and software modules, make the VESNA platform well suited for 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.

We continued to upgrade the LOG-a-TEC wireless sensor network testbed at the premises of Jožef Stefan Institute. In the Fed4FIRE (Federation for FIRE) project, the testbed was fully integrated in the Fed4FIRE federation by adopting the federation's interfaces and components and creating the necessary adapters. The testbed thus also became available to the community of external experimenters through a common Fed4FIRE portal. Furthermore, we designed a new architecture of sensor nodes, which will enable easier planning, deployment and debugging of user experiments and the remote collection of experimental data and results.

The LOG-a-TEC testbed was used and validated in the eWINE project for the performance evaluation of localization algorithms and for the investigation of radio spectrum occupancy in various frequency bands. Here, the emphasis was on effective covariance methods and their comparison with other methods of radio signal detection below 1 GHz. To this end we derived a methodology for a quantitative comparison of different spectrum sensing methods. In collaboration with SigFox we started the investigation of ultra-narrowband (UNB) radio signal detection in order to support the performance optimization and the increase of the density of low power wide area (LPWA) devices. We also prepared the first experimental architecture for UNB networks, which allows for the rapid development of experiments based on the data from physical and medium access control (MAC) layers.

As part of the work in eWINE we also developed a UWB radio channel classifier based on a convolutional neuron network approach, which determines (non) line-of-sight link conditions and hence the quality of the link using radio channel impulse response. The classifier was used as a support to increasing the indoor localization algorithm accuracy. The machine-learning approaches were also used in the design of a new link quality predictor for the wireless link quality estimation (LQE) based on measured signal strength (RSSI, received signal strength indicator) and the sequence of received data packets. The predictor can operate on the data obtained from different wireless technologies and enables the development of advanced MAC schemes and routing algorithms with the prioritization of channels. For the use in the LOG-a-TEC testbed the predictor was integrated into the ProtoStack tool used for service and protocol composition and reconfiguration.

In addition to the Fed4FIRE project, in 2016 we successfully concluded also CITI-SENSE project, in which we developed a VESNA-based portable device for air-quality monitoring via a smart user device (a phone or a tablet). The smart device was used for a graphical presentation of the measured data using the custom-developed mobile app and as a relay for sending raw data to a remote data server.

Finally, within the SUNSEED project we developed in collaboration with a company ComSensus two wide area measurement system (WAMS) devices for use in smart grids: one for the measurement of voltage and current phasors in real time (CP-SPM) and the other for the measurement of power quality and for the control of end devices (CP-PMC). We also actively participated in the deployment of these devices in the distribution network pilot of the project partner Elektro Primorska.

## Some outstanding publications in the past year

1. Gomez K., Javornik T., et al. Aerial base stations with opportunistic links for next generation emergency communications. *IEEE communications magazine*, [Print ed.], 2016, vol. 54, no. 4, pp. 31-39.
2. Kulin, M.; Fortuna, C.; De Poorter, E.; Deschrijver, D.; Moerman, I. Data-Driven Design of Intelligent Wireless Networks: An Overview and Tutorial. *Sensors* 2016, 16, 790.
3. Kourogiorgas C., Kelmendi A, Panagopoulos A. D., and Vilhar A. On rain attenuation time series generation: a new simple Copula-based channel model for satellite slant paths. *IEEE transactions on antennas and propagation*, ISSN 0018-926X. [Print ed.], 2016, vol. 64, no. 7, 3206-3211.
4. Trobec R., Vasiljević R., Tomašević M., Milutinović V., Bevide R., Valero M.. Interconnection networks in petascale computer systems : a survey. *ACM computing surveys*, 49(3), 2016, 44-1-44-24.

## Awards and appointments

1. Prof. Aleš Švigelj, dr. Kemal Alič, dr. Radovan Srncic: the Best Paper Award of the IEEE ComSoc Technical Committee on Communications Systems Integration and Modeling, "Network traffic modeling for load prediction: a user-centric approach", IEEE Network, IEEE Globecom 2016, Washington, USA, December 2016.

## Organization of Conferences, Congresses and Meetings

1. Nesus ECOST-MEETING-IC1305-070716-076861, Institut "Jožef Stefan", Ljubljana, 7-8. 7. 2016
2. SUNSEED 7th F2F meeting, Grand hotel Union, Ljubljana, 21.-22. 9. 2016

## INTERNATIONAL PROJECTS

- 7FP - CITI-SENSE; Development of Sensor-based Citizens' Observatory Community for Improving Quality of Life in Cities  
Prof. Mihael Mohorčič  
European Commission
- 7FP - ProaSense; The Proactive Sensing Enterprise  
Prof. Mihael Mohorčič  
European Commission
- 7FP - SUNSEED; Sustainable and Robust Networking for Smart Electricity Distribution  
Prof. Mihael Mohorčič  
European Commission
- 7FP - Fed4FIRE; Federation for FIRE - Federation for Future Internet Research and Experimentation  
Prof. Mihael Mohorčič  
European Commission
- 7FP - TETRACOM; Technology Transfer in Computing Systems  
Prof. Roman Trobec  
European Commission
- COST IC1405; Reversible Computation - Extending Horizons of Computing  
Prof. Monika Kapus Kolar  
Cost Office
- COST IC1305; Network for Sustainable Ultrascale Computing (NESUS)  
Prof. Roman Trobec  
Cost Office
- COST CA15104; Inclusive Radio Communication Networks for 5G and Beyond (IRACON)  
Asst. Prof. Tomaž Javornik  
Cost Office
- ESA - SatProSi-Alpha; Ka/Q-band Propagation Measurements and Modelling - Slovenian Contribution to the Alphasat TDP#5 Scientific Mission  
Dr. Andrej Vilhar  
Esa/estec.
- H2020 - eWINE; Elastic Wireless Networking Experimentation  
Prof. Mihael Mohorčič  
European Commission

## RESEARCH PROGRAMS

- Telecommunication Systems  
Prof. Mihael Mohorčič
- Parallel and Distributed Systems  
Prof. Roman Trobec

## R&D GRANTS AND CONTRACTS

- Model for Domain-Specific Trend Prediction based on Semantic Enrichment of Unstructured Patterns  
Prof. Roman Trobec
- Multi-analysis of fretting fatigue using physical and virtual experiments  
Prof. Roman Trobec
- Graph Optimisation and Big Data  
Dr. Matjaž Depolli
- Advanced Ray-Tracing Techniques in Radio Environment Characterization and Radio Localization  
Prof. Mihael Mohorčič
- Smart City Ecosystem - EkoSmart  
Prof. Roman Trobec

## NEW CONTRACTS

- Analysis of operational measures for prevention of ice formation on power lines  
Dr. Gregor Kosec  
Eles, d. o. o.
- Wearable Multifunctional Body Sensor (MedSens)  
Prof. Roman Trobec  
Simed d. o. o.
- Dynamic Thermal Rating of overhead power lines in icing conditions  
Dr. Gregor Kosec  
Eles, d. o. o.
- Advanced Ray-Tracing Techniques in Radio Environment Characterization and Radio Localization  
Prof. Mihael Mohorčič  
Xlab d. o. o.

## VISITOR FROM ABROAD

- Asst. Prof. Vesna Popović-Bugarin, Faculty of Electrical Engineering, University of Montenegro, 2.-7. 4. 2016
- Prof. Zoran Veljović, Faculty of Electrical Engineering, University of Montenegro, 2.-7. 4. 2016
- Asst. Prof. Enis Končan, Faculty of Electrical Engineering, University of Montenegro, 17.-31. 5. 2016
- Prof. Nermin Suljanović, Communications Department Faculty of Electrical Engineering Tuzla, Tuzla, Bosnia and Herzegovina, 30. 9. 2016
- Ao.Univ.-Prof. Dipl.-Ing. Dr. Erich Leitgeb, Institut für Hochfrequenztechnik / Institute of Microwave and Photonic Engineering Graz University of Technology, Graz, Austria, 30. 11. 2016

## STAFF

### Researchers

- Dr. Viktor Avbelj
- Dr. Carolina Fortuna
- Dr. Andrej Hrovat
- Asst. Prof. Tomaž Javornik
- Prof. Gorazd Kandus
- Prof. Monika Kapus Kolar
- Dr. Gregor Kosec
- Asst. Prof. Andrej Lipej\*
- Prof. Mihael Mohorčič, Head**
- Asst. Prof. Roman Novak
- Dr. Igor Ozimek
- Dr. Marjan Šterk, left 01.09.16*
- Prof. Aleš Švigelj
- Prof. Roman Trobec
- Dr. Andrej Vilhar

### Postdoctoral associates

- Dr. Kemal Alič
- Dr. Matjaž Depolli

- Dr. Aleksandra Rashkovska Koceva

### Postgraduates

- Klemen Bregar, B. Sc.
- Gregor Cerar, B. Sc.
- Urban Kuhar, B. Sc.
- Tomaž Šolc, B. Sc.
- Matevž Vučnik, B. Sc.

### Technical officers

- Polona Anžur, B. Sc.
- Miha Mohorčič, B. Sc.

### Technical and administrative staff

- Tomaž Krištofelc
- Vanessa Skvarča, B. Sc.
- Miha Smolnikar, B. Sc.
- Polonca Šega, B. Sc., left 05.01.16*

Note:

\* part-time JSI member



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1. A. G. Burr, Laurent Clavier, G. Dimic, Tomaž Javornik, Werner Teich, M. Mostafa, "Evolved physical layer", In: *Cooperative radio communications for green smart environments*, (River publishers series in communications, vol. 47), Narcis Cardona, ed., Gistrup, River Publishers, 2016, pp. 305-339.
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## MENTORING

1. Urban Gregorc, *Implementation of LoRa wireless communication for network of weather stations*: master's thesis, Ljubljana, 2016 (mentor Marko Jankovec; co-mentor Mihael Mohorčič).
2. Sebastijan Mrak, *Q-band (Ka-band) satellite receiver for observing Alphasat beacon*: master's thesis, Ljubljana, 2016 (mentor Matjaž Vidmar; co-mentor Andrej Hrovat).



# 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-adapting systems, 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 world-wide, through academic links and industrial contacts, thus enabling us to keep at the forefront of rapidly developing fields.*

Our research work in 2016 in the fields of efficient algorithms for massive-data processing, computing structures for faster and more reliable execution of algorithms, and interactive interfaces for the efficient acquisition and handling of data was enhanced by the design and development of various solutions within 11 European projects in Horizon 2020, ECSEL, ARTEMIS, FP7 and EEA Grants programs. We finished our work in the projects ACCUS, ENJOY IN HEALTH and TRUDEVICE. We continued with projects ISO-FOOD, REFRESH, RICHFIELDS, PD\_manager, MANTIS and EU Menu Slovenia. We started to work within three new projects ImAppNIO, SYNERGY and Trans fatty acids.

We were actively involved in the preparation of the JSI's application for strategic research innovative partnership (SRIP) in the field of **Smart Cities and Communities**, as a part of the Slovenian Smart Specialization Strategy. The application was positively evaluated and accepted for execution. The SRIP will allow enhancing the common execution of research and development programs of academic and industrial partners and will merge knowledge and competencies for the development of new products, services and processes.

### Computing Structures

In the field of advanced computer structures we continued the development of **self-reparable systems based on FPGA** and developed a platform for quick error penetration into the FPGA with the use of dynamic partial reconfiguration. The SRAM-based field-programmable gate arrays (FPGAs) in mission-critical systems require error mitigation and recovery techniques to protect them from single-event upsets (SEUs) and multiple-event upset (MEU) errors, caused by high-energy radiation. 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 an error-recovery mechanism in FPGA using dynamic partial reconfiguration were presented in the scope of our activities in the COST *Action IC1204 TRUDEVICE - Trustworthy Manufacturing and Utilization of Secure Devices* (<http://trudevice.com/>).

Within the TRUDEVICE project we studied the **security upgrade of the IEEE Std 1149.1 scan design chains** also known as the JTAG standard. The JTAG scan chains are designed to enhance the system's testability and can potentially be used to break in a system and steal intellectual property or perform some other malicious action. The risk of system break-in should be seriously considered and appropriate countermeasures taken. We have analysed currently proposed solutions and pointed out some problems of adding decoding and encoding logic to scan chains as a possible countermeasure. Besides non-negligible logic overhead, this solution requires special software provided by the ASIC vendor for the proper interpretation of the scan test results. The security extension of the JTAG standard aims to prevent unauthorized users from breaking into a system and disturbing its normal operation via IEEE 1149.1 test port. For this solution, a possible attack scenario was described and probabilities that the system gets compromised within a certain time frame were calculated, together with the lower bound values of the Lock register length that ensure the required system security. In the frame of ECSEL JU *MANTIS - Cyber Physical System based Proactive Collaborative Maintenance* (<http://www.mantis-project.eu/>) we are currently exploring modifications to the locking mechanism, including different PKI architectures, which would allow different authorization levels, and possibly also the change of authorization keys.

In the field of **embedded systems** we developed a new generation of portable BLE kitchen scale with a low power consumption. The scale consists of a communication module built of the BLE113 interface that connects



Head:

**Asst. Prof. Gregor Papa**

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**We developed procedures for the optimal broadcasting of multiple messages in networks.**

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other parts of the scale, also allowing a power-save mode, and a measurement module that is built around the measurement bridge and an accurate AD converter. For enhancing the battery life, the measurement module turns off when the scale is in standby mode.

We developed a **Bluetooth Low Energy (BLE) sensor network** with a communication mechanism that enables the data acquisition from distant nodes using intermediant BLE sensor nodes as the relays. BLE is a communication technology developed for low-power-consumption and low-cost applications. However, the BLE supports only simple communication schemes and does not support the creation of the communication network. Since the range of the BLE devices is relatively small some sensor nodes can become unavailable from the central acquisition system. To overcome this BLE limitation a new communication mechanism was developed for the BLE sensor node to relay the data from other nodes. This is achieved by switching the role of the intermediant node from a slave to a master, gathering the data from other intermediant and/or leaf nodes, and reporting all the data to its master. A hardware prototype to validate the implemented mechanism was developed.

In the scope of **sensors** research we studied the effect of a temporary presence of liquids that may importantly influence the response of a LTCC-based pressure sensor in a Wheatstone bridge configuration. A specific time response of offsite voltage was observed during the experimentation with droplets of water dispensed on the diaphragm. Such a response may result from the dynamic changes in the temperature distribution due to the local cooling caused by the evaporation of the liquid covering the sensing diaphragm. Based on this assumption an FE model is under development, in which heat transfer resulting from the evaporation of the liquid film was defined as a discrete function of time. An initial FE analysis confirms the trends of experimental measurements.

#### Algorithms for Data Processing

Our research in the field of efficient algorithms for computer data processing was focused on the development of multi-objective optimization approaches, the study of optimal information transfer in networks and pattern recognition. Some solutions were used on the application level within computer support for diet planning and our Open platform for clinical nutrition (OPEN). Here we can highlight the algorithms for food matching, for the automatic recognition and detection of food and drinks from images by using deep learning, and applications for

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**We are developing an algorithm for the automatic detection and recognition of food and drinks from images by using a deep-learning technique.**

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computer-assisted dietary assessment, weight-loss programmes, and tracking the physical activity of children and teenagers with sport wristbands.

To improve our excellence and unleash research and innovation potential in the field of **multi-objective optimization, supported by parallelisation and surrogate modelling** we started a Twinning project Horizon 2020 SYNERGY - *Synergy for smart multi-objective optimisation* (<http://synergy-twinning.eu/>), which we are also coordinating. In the project we are collaborating with the Department of Intelligent Systems at JSI, Cologne University of Applied Sciences (CUAS), and University of Lille (USTL). The goal of the project is to overcome the limitations of the current initial-stage research in multi-objective optimization at the Jožef Stefan Institute, where efficiency measures have only been explored on a very small scale and with no collaboration with other partners. USTL is a leading partner in parallelisation on large-scale heterogeneous architectures, while CUAS provides expertise in surrogate modelling and its deployment in optimisation problems. In 2016 we have carried out several visits to the participating partners, and conducted several joint workshops at renowned international conferences for the needs of education in the framework of the project.

We researched **optimal broadcasting of multiple messages** – in terms of time and the number of messages – in the 1-in port model, where every vertex of a synchronous network can receive at each time unit at most one message. We considered simultaneous broadcasting of multiple messages from the same source in such networks with an additional restriction that every received message can be sent out to neighbours only in the next time unit and never to an already informed vertex. We used a general concept of level-disjoint partitions developed for this scenario. We provided a necessary condition in terms of girth and eccentricity of the root for the existence of  $k$  same-rooted level-disjoint partitions of optimal height and provided a structural characterization of graphs that admit simultaneous broadcasting of two messages from a given vertex. We introduced a subgraph extension technique for efficient information spread within the concept of a level-disjoint partition. This approach, with so-called biwheels, leads to the simultaneous broadcasting of the optimal number of messages on a wide class of graphs in an optimal time. In particular, we provided tight results for bipartite tori, meshes, and hypercubes. We successfully presented our results at the COCOA 2016 conference.

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We introduced a **new measure for a balanced workload** and we determined its extremal values as well as the graph structures where the extremal values are attained. To measure the extent to which the distribution of the workload in the network can be equalized, a degree-weighted measure for a balanced workload based on betweenness centrality was introduced. The goal was to determine the extremal values of the measure, and the structures where these values are attained.

To work on a **mathematical formalization of artificial genetic representations with neutrality**, a visit to the University of Coimbra was made. The visit was supported by COST Action *ImAppNIO - Improving Applicability of Nature-Inspired Optimisation by Joining Theory and Practice* (<http://imappnio.dcs.aber.ac.uk/>). The potential that neutral networks have to establish alternative paths for the evolution of the population, and to lead to improved search quality, is the main motivation for the use of redundant representations in evolutionary computation. The role of neutrality in evolutionary search has been widely considered in the literature, but it remains unclear to what extent it may contribute to the search performance. In studies, a promising class of representations based on error-control codes was proposed, leading to families of representations with various degrees of neutrality, synonymy, connectivity, and locality.

Within the European ARTEMIS association we successfully finished our work in the project *ACCUS - Adaptive Cooperative Control in Urban (sub) Systems* (<http://www.projectaccus.eu>), where we collaborated in the development of 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 the combined performance. We upgraded the **traffic-flow simulation framework**, based on the OpenDRIVE logical description of a road network. The framework includes the descriptions of the road network and the traffic lights and allows the simulation of vehicle flows, according to the IDM (Intelligent driver model). It allows simple and intuitive planning of new and/or changed road segments, since their influence can be easily observed. The upgraded simulator also allows the optimization of traffic lights' switch segments, resulting in more fluent traffic flows.

In the area of **pattern recognition** we studied electrocardiographic indices as a function of the coupling interval and the site of ventricular premature beats, in an isolated rabbit heart preparation using electrocardiographic multi-lead system. In both ventricles, results have shown significant increases in ventricular depolarization duration. We have also observed that when the ventricular premature beats were applied to the left ventricle, a significant decrease in the total repolarization duration was detected, while the right ventricle premature stimulation has not exhibited significant changes in the total repolarization duration. We compared twenty machine-learning classification techniques to find the optimal electrode placement for the left and the right ventricle stimulation and to interpret the site of the origin of ventricular premature beats.

The Horizon 2020 project *RICHFIELDS - Research Infrastructure on Consumer Health and Food Intake for Esience with Linked Data Sharing* (<http://www.richfields.eu/>) is focused on food- and nutrition-related data. The main aim of the project is to design the architecture of a platform for collecting, linking and harmonizing big and open data provided by various information systems and mobile apps. In a pilot, which aims to identify gaps and problems in the area of food composition data, we have developed an advanced **algorithm for matching food items** indexed and classified by using different standards, such as LanguaL and FoodEx2. The algorithm is based on POS tagging, also developed at our department. We presented the approach at the Food Forum 2016 in Brussels. The approach was recognized as the most promising among all the approaches presented by European institutions. A similar approach was used in another project *EU Menu - Support to National Dietary Surveys in Compliance with the EU Menu methodology*, co-financed by the European Food Safety Agency EFSA. This project aims at collecting data on food consumption habits and patterns across Slovenia. Food-consumption data are essential for assessing how exposed people are to potential risks in the food chain. In cooperation with the Slovenian Public Health Institute (NIJZ) we developed a mobile app for 24h recall. The app is based on the food consumption data managed by the OPEN. To enable data transmission to EFSA, the application has been upgraded with web services. Within this project, OPEN has also been extended to support the **statistical analysis of collected data**.

Another Horizon 2020 project *PD\_manager - mhealth platform for Parkinson's disease management* (<http://www.parkinson-manager.eu/>) aims at developing a set of unobtrusive and co-operative mobile devices that will be used by Parkinson's disease patients for symptoms monitoring and the collection of adherence data. As Parkinson's disease patients also have nutritional problems, such as dysphagia and constipation, and may experience side-effects of some food on drugs, we have developed a nutrition mobile application for food, drinks and drug tracking. The application is based on the automatic recognition of food and drinks from images taken by a patient or his caregiver with a smartphone. The **recognition algorithm is implemented by deep-learning techniques**. Preliminary results were



Figure 1: Mobile application for traffic routing and navigation.



Figure 2: User interfaces of mobile apps for people with Parkinson's disease.

presented at the international conference organized by the Slovenian society for dysphagia in Ljubljana in May (<http://disfagija.si/sl/home/>).

The project *ENJOY IN HEALTH – Celostni inovativni model za zagotavljanje zdravega življenjskega sloga, s poudarkom na prehranjevanju, gibanju, preprečevanju in obravnavi debelosti pri otrocih, mladostnikih ter odraslih in zmanjševanju neenakosti v zdravju* (<http://uzivajmovzdravju.si>) was financed by the Norway Financial Mechanism. The main objective of the project was to decrease and prevent unhealthy lifestyle-related diseases. The project outcomes included the development and testing of inter-disciplinary prevention teams within the education sector, health/medical sector, social sector and the local communities with the aim to support a healthy lifestyle; and innovative intervention programmes for the non-medicinal treatment of obesity for children, youth and adults. In cooperation with the NIJZ, our department developed a **web-based and a mobile app for assisting a weight-loss programme** performed by the Slovenian health homes. In a pilot, the app was tested in 12 health centres. Another output was a mobile app Fitus aimed at tracking the physical activity of children and teenagers using a wristband. Data about the user's activity and heart rate measured by the wristband are stored in a cloud, which can be accessed by the app via an API. The app tracks the development of the pupil's performances through periods. As the application is also connected by the OPEN, it enables a statistical analysis of collected data as well as a link of data about physical activity and heart rate with data about dietary habits.

Our department is a partner in the consortium of the ARRS applied project *Trans fatty acids*, financed by ARRS. In the first period of the project, groups of pre-packaged foods that are potentially most significant sources of trans fatty acids (TFA) were identified and the content of TFA in vegetable fats was analysed. Our department contributed to the estimation of the intake of TFA in the most risky population group, i.e., students consuming subsidized student food. The estimation was performed by using data on the TFA content in foods collected in database of the **Open platform for clinical nutrition**. The results were published in <http://www.delo.si/prosti-cas/zdravje/nutricionisti-bi-vsebnost-trans-mascob-v-zivilih-zakonsko-omejili.html>.

In the Horizon 2020 project *REFRESH – Resource Efficient Food and dRink for the Entire Supply cHain* (<http://eu-refresh.org/>) we will contribute towards the objectives of reducing food waste across Europe by 30 % by 2025, reducing waste-management costs, and maximizing the value from unavoidable food waste and packaging materials. We are developing a database of unavoidable food waste.

In cooperation with the *Milko Kos Historical Institute of ZRC SAZU* we worked on the new portal Slovenian Historical Topography. The long-term goal will be to produce a thorough and reliable **digital interactive version of historical topography of the entire territory of the present-day Republic of Slovenia**. The first step in this objective has already been successfully achieved by the project *Slovenian place-names in time and space*, which covered the territory of the historical province of Carniola. The original printed handbook from 1975 was thus replaced with an up-to-date interactive web application with advanced search possibilities, geolocation, connection of database with online geographical map and a circa 30 % richer – updated and corrected – database (<http://topografija.zrc-sazu.si/>).

Applying our research results, we developed a **web-based tool for the e-learning of statistics**. This tool is primarily aimed to be used by the ERA Chair ISO-FOOD for distance teaching chemistry and physics students. It leads the student in using different methods for statistical analysis. Currently, we are performing the testing of the tool in

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### We have developed an e-learning tool for statistics.

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collaboration with the *Department of Environmental Sciences* at the JSI.

To improve the department's excellence in the field of statistics, we launched a series of **statistical seminars**. The seminars are conducted on a weekly basis and are intended for the staff and associates of the department. The seminars are on two levels. The basic statistical seminar is meant to refresh and deepen the basic knowledge of statistics. It is carried out in the form of the lectures and it follows the curriculum of statistics at Slovenian universities. The advanced group is intended to upgrade their basic knowledge of statistics and study the advanced topics of statistics and machine learning. Our aim is to extend the work of the seminar beyond the boundaries of the department.

In cooperation with the *Department of Intelligent Systems* at the JSI we organized in May the BIOMA 2016 conference Bioinspired Optimization Methods and their Applications (<http://bioma.ijs.si/conference/2016/>). The seventh biennial conference included the presentations and discussions on the newest theoretical and practical results on nature-inspired optimization methods and their applications. The presentations are included in the conference proceedings.

In cooperation with the *Department of Intelligent Systems* at the JSI and the *Faculty of Electrical Engineering and Computer Science, University of Maribor* (Laboratories for Computer Architecture and Languages and Programming Methodologies), we organized, for the thirteen consecutive year, the **workshops on Nature-inspired algorithms** on stochastic optimization techniques.

### Human-Computer Interaction

In the area of efficient interaction systems, we focused on a study of **usage scenarios** within human-machine interaction, we developed **serious games** for telerehabilitation, and we continued with development and usage of recognized **procedures and tools for usability testing**.

Our work in the MANTIS project was focused on the **design and development of human-machine interaction**. Following a user-centred design paradigm, our early work comprised gathering the MANTIS system use scenarios from industrial partners, which serve as a cornerstone for the design of intelligent and context-aware user interface for proactive and collaborative maintenance. From the gathered use scenarios, we were deriving requirement specifications for human-machine interaction and developing an interaction model that supports proactive maintenance, collaboration among the users, collaboration between the users and the MANTIS system, and includes context-aware functionalities. In addition, we contributed to the description and representation of different interface types, and the preparation of the guidelines for interface design. We have already started with the implementation of a user-interface prototype.

Within the Horizon 2020 project PD\_manager we also developed and implemented the **gamification of physiotherapy for people with Parkinson's disease**. The aim was to show how off-the-shelf equipment could be used to develop serious games for an affordable tele-medicine solution for Parkinson's disease management. Two games have been developed in collaboration with the *Soča rehabilitation institute* aimed at assessing and training a patient's reach of upper limbs (using Kinect v2) and fine motoric skills of fingers (using Leap motion). The games collect player data

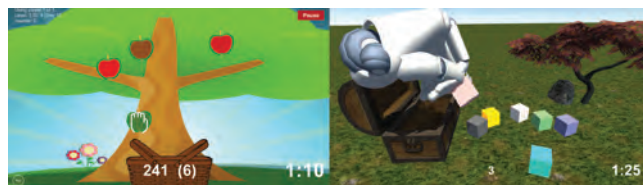


Figure 3: Serious games for the rehabilitation of people with Parkinson's disease.

in terms of the score achieved and the full kinematics of movement during gameplay. The games have been tested with patients within the Soča rehabilitation institute as well as at their homes. We also designed and developed the server side of the system, which consists of a database to store anonymized user data, game scores and kinematic data. It is also used as a service to share data among different client machines and as user interface for clinicians.

In cooperation with the informal community *Slovenian human-computer interaction researchers* (<http://hci.si/>), we organized the 3rd Human-Computer Interaction in Information Society (HCI-IS) conference in October (part of the Information society multiconference). This year's edition saw an increase of attendance from the previous years with contributions from academia and industry. The main purpose of the event is to connect Slovenian researchers interested in HCI in order to exchange ideas, collaborate and accelerate the development of this exciting interdisciplinary field in Slovenia and its surrounding countries. Here, we also reported a usability testing of the graphical user interface of the GUARD simulator developed by Guardiaris d.o.o. This BSc thesis was supervised by a member of our department.

We redesigned the Slovenian avalanche bulletin (<http://www.meteo.si/pozor/plaz>), of the Slovenian environment agency, with a **usability study of the proposed prototypes**. The study informed the agency about which version is better understood by different user groups and what are their comments. Besides usability, the educational aspect of the bulletin was also taken into consideration. The undertaken testing was a mixture of exploratory and evaluation study aimed at gathering qualitative data. Together with the client, we defined the goals of the study and the questions that the study needs to answer. We then prepared scenarios with tasks that the users performed during testing. After testing and an online survey, the results were analysed and a set of findings and list of possible improvements was given to the client.

Within the TETRACOM *PerNuCAP - Personalized Nutrition Control Aid for Insulin Patch Pump*, we conducted **usability testing of the Insulin Patch Pump** developed by IPDmed company. Following the *Usability Testing of Medical Devices* IEC 62366 standard. We carried out the introductory



Figure 4: Usability study to support the redesign of the Slovenian avalanche bulletin.

study of the purpose and intended use of the pump, intended user population and conditions of use. We examined the functionalities of the device and the risk analysis already conducted by IPDmed. From the preceding studies we specified the comprehensive list of the primary operating functions, i.e., frequently used functions and functions, related to the safety of the device. We also identified possible use scenarios and user actions for each function.

The PD\_manager platform consists of different modules with different interfaces (web, mobile, natural) and different users. The most sensible ones are the modules that interface with the patients. To ensure accessibility of all the interfaces with the patients, we started a usability study of how patients with Parkinson's interact with the PD\_manager platform. In addition, to study **user experience design** we defined the visual language for the project's user interfaces and redesigned the mobile interfaces accordingly. The case study for the new visual language was a mobile app for tracking nutrients and foods consumed by patients with Parkinson's disease. The new interface



allows the patients to recognize objects on the screen, easily perceive their function and interact with them, thus providing an efficient way of entering the dietary intake data.

We conceived UsabEU to provide a **web-based starting point for usability evaluations** with questionnaires in native or mother tongue. We designed a platform that supports the online collaborative translation of usability questionnaires and their validation. It also serves as a repository for all validated questionnaires and a tool to perform usability evaluations. The current proof-of-concept design of the platform supports the translation and validation of the System Usability Scale questionnaire.

### Some outstanding publications in the past year

1. A. Kostevšek, J. Klemeš, P. Varbanov, G. Papa, J. Petek, "The concept of an ecosystem model to support the transformation to sustainable energy systems", *Applied energy*, 184: 1460 – 1469, 2016, doi: 10.1016/j.apenergy.2016.04.010.
2. P. Gregor, R. Škrekovski, V. Vukašinović, "Time-optimal broadcasting of multiple messages in 1-in port model", *Combinatorial optimization and applications: 10th International Conference, COCOA 2016, Lecture notes in computer science*, 10043: 144-158.
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4. P. Vrtič, M. Vražič, G. Papa "Design of an axial flux permanent magnet synchronous machine using analytical method and evolutionary optimization", *IEEE transactions on energy conversion*, 31: 150-158, 2016, doi: 10.1109/TEC.2015.2477319.
5. A. Biasizzo, F. Novak, "Security problems of scan design and accompanying measures", *Journal of electrical engineering*, 67: 192-198, 2016.

### Organization of conferences, congresses and meetings

1. AVN, The 28th Workshop Nature-Inspired Algorithms, Bled, Slovenia, 18. 5. 2016
2. SYNERGY project-meeting, Bled, Slovenia 18.–19. 5. 2016
3. MANTIS, full consortium project-meeting, Ljubljana, Slovenia 17.–20. 5. 2016
4. BIOMA 2018, The 7th International Conference on Bioinspired Optimization Methods and their Applications, Bled, Slovenia, 18.–20. 5. 2016
5. HCI-IS 2016, Conference Human-Computer Interaction in Information Society, Ljubljana, Slovenia 9. 10. 2016
6. AVN, The 29th Workshop Nature-Inspired Algorithms, Maribor, Slovenia, 2. 12. 2016

### Patent granted

1. Gregor Papa, Barbara Koroušič-Seljak, Marko Pavlin, Device and method for acquisition and transfer of signals, SI24792 (A), Slovenian Intellectual Property Office , 29. 02. 2016.

## INTERNATIONAL PROJECTS

1. 7FP - TETRACOM; Technology Transfer in Computing Systems  
Prof. Franc Novak  
European Commission
2. Adaptive Cooperative Control in Urban (sub) Systems  
Asst. Prof. Gregor Papa  
Ministrstvo za Gospodarstvo
3. 7 FP; ERA CHAIR ISO-FOOD - Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability  
Asst. Prof. Barbara Koroušič Seljak  
European Commission
4. EU MENU Slovenija; LOT 1; Support to National Dietary Survey in Compliance with the EU MENU Methodology - Fourth Support  
Asst. Prof. Barbara Koroušič Seljak  
European Food Safety Authority - Efsa
5. EU MENU Slovenija; LOT 2; Support to National Dietary Survey in Compliance with the EU MENU Methodology - Fourth Support  
Asst. Prof. Barbara Koroušič Seljak  
European Food Safety Authority - Efsa
6. COST IC1204; Trustworthy Manufacturing and Utilization of Secure Devices  
Prof. Franc Novak  
Cost Office
7. COST CA15140 - ImAppNIO; Improving Applicability of Nature-Inspired Optimisation by Joining Theory and Practise  
Dr. Vida Vukašinović  
Cost Office
8. H2020 - MANTIS; Cyber Physical System based Proactive Collaborative Maintenance

Asst. Prof. Gregor Papa  
European Commission

9. H2020 - REFRESH; Resource Efficient Food and Drink for the Entire Supply Chain  
Asst. Prof. Barbara Koroušič Seljak  
European Commission
10. H2020 - RICHFIELDS; Research Infrastructure on Consumer Health and Food Intake using E-science with Linked Data Sharing  
Asst. Prof. Barbara Koroušič Seljak  
European Commission
11. H2020 - PD\_manager; Mhealth Platform for Parkinson's Disease Management  
Asst. Prof. Barbara Koroušič Seljak  
European Commission
12. H2020 - SYNERGY; Synergy for Smart Multi-Objective Optimisation  
Prof. Peter Korošec  
European Commission

## RESEARCH PROGRAM

1. Computer Structures and Systems  
Asst. Prof. Gregor Papa

## R & D GRANTS AND CONTRACTS

1. Advanced electrocaloric energy Conversion  
Asst. Prof. Barbara Koroušič Seljak

- Norway Grants „Enjoy in Health“: An Integrated Innovative Model for the Provision of a Healthy Lifestyle, with a Focus on Nutrition, Physical Activity, Obesity Prevention and Treatment in Children, Adolescents and Adults and  
Asst. Prof. Barbara Koroušič Seljak  
Republic of Slovenia, Government Office for Development and European Cohesion Policy
- Adaptive Cooperative Control in Urban (sub) Systems  
Asst. Prof. Gregor Papa  
Republic of Slovenia, Ministry of Economic Development and Technology
- 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  
Eurofir Aisbl
- Conference BIOMA 2016; The 7th International Conference on Bioinspired Methods and their Applications, Bled, Slovenia, 18.-20.05.2016  
Asst. Prof. Gregor Papa
- Electronic Questionnaire; Data Collection and Monitoring about Gastrointestinal Symptoms  
Asst. Prof. Barbara Koroušič Seljak  
Espghan Office

## NEW CONTRACTS

- Personalized Nutrition Control Aid for Insulin Patch Pump – PerNuCAP  
Prof. Franc Novak  
IpD Med d. o. o.

## VISITORS FROM ABROAD

- Thomas Bartz Beielstein, Boris Naujoks, Jörg Stork, Technische Hochschule Köln, Germany, 10.-11. 2. 2016
- Nouredine Melab, El-Ghazali Talbi, Universite des Sciences et Technologies de Lille I, Lille, France, 10.-11. 2. 2016
- Thomas Bartz Beielstein, Boris Naujoks, Technische Hochschule Köln, Germany, 17.-20. 5. 2016
- Nouredine Melab, El-Ghazali Talbi, Universite des Sciences et Technologies de Lille I, Lille, France, 17.-20. 5. 2016
- Goran Martinović, Fakultet elektrotehnike, računarstva i informacijskih tehnologija Osijek (FERIT) Osijek, Croatia, 17.-20. 5. 2016
- Roberto Uribeetxeberria, Urko Zurutuza, Mondragon Unibertsitatea, Faculty of Engineering, Arrasate-Mondragon, Spain, 23.-25. 5. 2016
- Roberto Gonzalez, Fundacion Tekniker, Eibar, Spain, 23.-25. 5. 2016
- Salvatore Esposito, Mario Riccardi, Ansaldo STS, Genova, Italy, 23.-25. 5. 2016
- Stanislava Velkova, 3E, Brussels, Belgium, 23.-25. 5. 2016
- Erkki Jantunen, Teknologian tutkimuskeskus VTT, Espoo, Finland, 23.-25. 5. 2016
- Antti Niemela, Lapin Ammattikorkeakoulu, Kemi, Finland, 23.-25. 5. 2016
- Bas Tjisma, Philips Consumer Lifestyle, Drachten, Netherlands, 23.-25. 5. 2016
- Jerker Delsing, Luleå University of Technology, Department of Computer Science, Electrical and Space Engineering, Luleå, Sweden, 23.-25. 5. 2016
- Marjan Šterk, XLAB, Ljubljana, Slovenia, 23.-25. 5. 2016
- Boris Naujoks, Technische Hochschule Köln, Germany, 10.-11. 11. 2016

## STAFF

### Researchers

- Asst. Prof. Anton Biasizzo
- Prof. Peter Korošec
- Asst. Prof. Barbara Koroušič Seljak
- Prof. Stanislav Kovačič\*
- Prof. Franc Novak
- Asst. Prof. Gregor Papa, Head
- Asst. Prof. Jurij Šilc

### Postdoctoral associates

- Dr. Bojan Blažica
- Dr. Marko Pavlin\*
- Dr. Drago Torkar

- Dr. Vida Vukašinović

### Postgraduates

- Rok Hribar, B. Sc.
- Martin Pečar, B. Sc.

### Technical officers

- Špela Poklukar, B. Sc.

### Technical and administrative staff

- Jolanda Jakofčič

Note:

\* part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

- Anton Biasizzo, Franc Novak, "Security problems of scan design and accompanying measures", *J. Elektr. Eng.*, vol. 67, no. 3, pp. 192-198, 2016.
- Jelena Klisara, Riste Škrekovski, Vida Vukašinović, Damir Vukičević, "A measure for a balanced workload and its extremal values", *Discrete appl. math.*, vol. 200, pp. 59-66, 2016.
- Anja Kostevšek, Jiri Klemeš, Petar Varbanov, Gregor Papa, Janez Petek, "The concept of an ecosystem model to support the transformation to sustainable energy systems", *Appl. energy*, vol. 184, pp. 1460-1469, 2016.
- Matej Kristan, Vildana Sulić Kenk, Stanislav Kovačič, Janez Perš, "Fast image-based obstacle detection from unmanned surface vehicles", *IEEE trans. cybern.*, vol. 46, no. 3, pp. 641-654, Mar. 2016.
- Peter Vrtič, Mario Vražič, Gregor Papa, "Design of an axial flux permanent magnet synchronous machine using analytical method and evolutionary optimization", *IEEE trans. energy convers.*, issue 1, vol. 31, pp. 150-158, mar. 2016.

## PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

- Gregor Papa, Urko Zurutuza, Roberto Uribeetxeberria, "Cyber physical system based proactive collaborative maintenance", In: *Proceedings of 2016 International Conference on Smart Systems and Technologies, (SST), Osijek, Croatia, October 12-14, 2016*, pp. 173-178.

## PUBLISHED CONFERENCE CONTRIBUTION

- Simon Beltram, Gregor Papa, "Optimizacija geometrije profila letalskega krila", In: *Zbornik petindvajsete mednarodne Elektrotehniške in računalniške konference ERK 2016, 19. - 21. september 2016, Portorož, Slovenija*, (Zbornik ... Elektrotehniške in računalniške konference ERK ..., 25), zv. B, pp. 75-78.
- Bojan Blažica, Franc Novak, Anton Biasizzo, Ciril Bohak, "3D serious games for Parkinson's disease management", In: *Interakcija človeka-računalnik v informacijski družbi: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 11. oktober 2016, [Ljubljana, Slovenija]: zvezek E*, pp. 9-12.

3. Tome Eftimov, Peter Korošec, Barbara Koroušič-Seljak, "Disadvantages of statistical comparison of stochastic optimization algorithms", In: *Bioinspired optimization methods and their applications: proceedings of the Seventh International Conference on Bioinspired Optimization Methods and their Applications - BIOMA 2016, 18-20 May 2016, Bled, Slovenia*, pp. 105-118.
4. Tome Eftimov, Peter Korošec, Barbara Koroušič-Seljak, "Knowledge extraction of evidence - based dietary recommendations", In: *Zbornik*, 8. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana, 31. maj in 1. junij 2016, Ljubljana, Slovenija, pp. 149-153.
5. Dimitros Gatsios, George Rigas, Dragana Miljković, Barbara Koroušič-Seljak, Marko Bohanec, María Soledad Arredondo, Angelo Antonini, Spyros Konitsiotis, Dimitrios I. Fotiadis, "Mhealth platform for Parkinson's disease management", In: *Final program*, CBHI 2016, 18th International Conference on Biomedicine and Health Informatics, Februar 25-26, Dubai, UAE, 5 pp..
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8. Peter Novak, Barbara Koroušič-Seljak, Franc Novak, "Designing visual interface for nutrition tracking of patients with Parkinson's disease", In: *Interakcija človek-računalnik v informacijski družbi: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 11. oktober 2016, [Ljubljana, Slovenija]: zvezek E*, pp. 13-16.
9. Gal Pavlin, Marko Pavlin, "Towards affordable mobile crowd sensing device", In: *Interakcija človek-računalnik v informacijski družbi: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 11. oktober 2016, [Ljubljana, Slovenija]: zvezek E*, pp. 37-39.

10. Drago Torkar, Pedro David Arini, "Analysis of an electrocardiographic multilead system by means of artificial neural networks, Study of repolarization during premature ventricular stimulation", In: *BIOSTEC 2016: proceedings*, (Biosignals, volume 4), 9th International Joint Conference on Biomedical Engineering Systems and Technologies, February 21 - 23, 2016, Rome, Italy, pp. 34-41.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Barbara Koroušič-Seljak, E. Vasco, Paula Alvito, "OPEN platform for clinical nutrition - an online dietary assessment: an online dietary assessment", In: *Food contaminants and human health: challenges in chemical mixtures*, pp. 63-66.

## SCIENTIFIC MONOGRAPH

1. Miha Kosi, Matjaž Bizjak, Miha Seručnik, Jurij Šilc, *Historična topografija Kranjske (do leta 1500)*, (Slovenska historična topografija, 1), 1. e-izd., Ljubljana, Založba ZRC, 2016.

## PATENT

1. Gregor Papa, Barbara Koroušič-Seljak, Marko Pavlin, *Device and method for acquisition and transfer of signals*, SI24792 (A), Urad RS za intelektualno lastnino, 29. 02. 2016.

## MENTORING

1. Anja Gaber, *Design and evaluation of the nutritional profile of gluten-free foods*: master's thesis, Ljubljana, 2016 (mentor Marjan Simčič; co-mentor Barbara Koroušič Seljak).
2. Andraž Škoda, *Detection of surface defects on highly glossy objects*: master's thesis, Ljubljana, 2016 (mentor Stanislav Kovačič).

# DEPARTMENT OF KNOWLEDGE TECHNOLOGIES

# E-8

*Department of Knowledge Technologies performs research in advanced information technologies aimed at acquiring, storing and managing knowledge to be used in the development of an information- and knowledge-based society. Established areas of our work include intelligent data analysis (machine learning, data mining, and knowledge discovery in databases), language technologies and computational linguistics, computational creativity, decision support and knowledge management. In addition to research in knowledge technologies, we are also developing applications in environmental sciences and management, agronomy, medicine, biomedicine and bioinformatics, economics, finance and marketing. The department is also a recognised centre for linguistic research and digital humanities.*

In 2016 we were involved in twelve national projects, eight EU FP7 and four Horizon 2020 projects, one COST action, two bilateral projects, one infrastructure project and four industry projects. The department hosted nine junior researchers working towards their PhDs.

In the area of **intelligent data analysis and data mining** we have developed several new methods and used them in a number of application domains. In the area of semantic data mining we have developed a method for explaining mixture models through semantic pattern mining and banded matrix visualization, published in the respected Machine Learning journal and a method for network-ranking-assisted semantic data mining. In the area of heterogeneous network analysis we developed new search-heuristics-based text mining. We continued work in the area of multi-view clustering using multi-target predictive clustering trees, with a similar method applied to clustering of Alzheimer's disease patients. A new web platform for text mining and natural language processing TextFlows was developed, together with complex language processing workflows, and presented in the Science of Computer Programming journal. In text mining we continued research in bisociative cross-domain link discovery. Within the PD\_manager project, which we coordinate at JSI, we developed a multi-view methodology for determining groups of patients with similar symptoms and detecting patterns of medication changes that lead to the improvement or decline of patients' quality of life.

We have developed new methods for the automated modelling of dynamic systems, using both data and domain knowledge, and have applied them to problems in the areas of environmental and life sciences. These include methods for learning ensembles of deterministic process-based models and methods for learning stochastic process-based models. We have adapted the methods for learning process-based models for the task of designing dynamic biological systems and demonstrated their utility on several problems from synthetic biology.

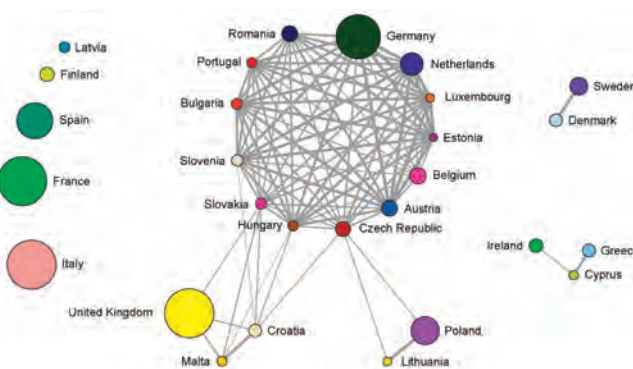
We are coordinating the FP7 FET project MAESTRA (Learning from Massive, Incompletely Annotated, and Structured Data), which focuses on analysing data that may be complex in several ways. Within MAESTRA we have developed many new methods for structured output prediction in a batch or streaming setting. These include methods for multi-target regression, such as learning option trees in batch setting, as well as learning trees and tree ensembles in streaming setting. The latter have been used to perform multi-label classification on data streams. We have also developed methods for feature ranking for different types of structured outputs. Finally, we have proposed a method to organize the labels in multi-label classification into a hierarchy, which improves the predictive performance.

We have used methods of predictive clustering for the analysis of various aspects of the biology of extremophilic fungi, which can act as opportunistic human pathogens. We have also used these methods for the identification of multi-output dynamic systems in batch and streaming settings. Finally, we used methods for multi-target regression in the ESA Mars Express Power Challenge, where the task was to predict the power consumption of 33 different lines of the thermal subsystem for the Mars Express orbiter.



Head:  
**Prof. Nada Lavrač**

**Our team won the ESA's Mars Express Power Challenge, designing the most accurate solution for predicting a space probe's power consumption.**



*Figure 1: A network of the EU countries, linked by tweet sharing. The size of a node is proportional to the number of EP members from that country. The network contains one large connected component consisting of 18 countries, with a core of 13 countries around Germany that are densely connected.*

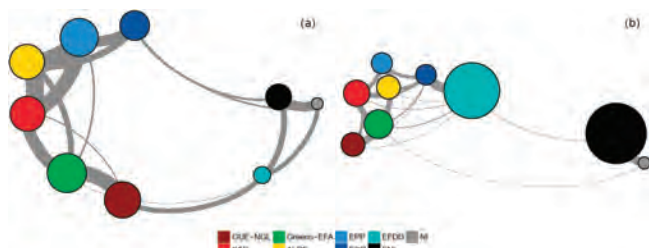


Figure 2: Networks of roll-call votes and retweets. (A) Co-voting agreement within and between political groups in the EP. (B) Average retweets within and between political groups.

In the context of the FET Flagship HBP (Human Brain Project) project, we are developing new data-mining methods and applying them to discover biological signatures of neurodegenerative diseases, such as Alzheimer's and Parkinson's. A new multi-view clustering method was developed and used for the identification of gender-specific biomarkers for Alzheimer's disease. Several methods for redescription mining, based on predictive clustering, were developed and applied to data on Alzheimer's disease. Finally, we have applied predictive clustering trees to relate biomarkers and clinical scores for Parkinson's disease.

In collaboration with the French Institute ARVALIS (Institut du végétal), we launched the project BIODIV (Understanding and managing biodiversity in agricultural ecosystems by data mining and decision support). We organized a workshop where we explored the current state of data collection and the modelling of habitats and population dynamics for auxiliary species that perform biological control of pests (such as aphids) in cereal crops. We performed extensive and complex data pre-processing, grouping organisms into functional categories and linking sampling sites to their environmental characteristics, thus getting ready to apply data mining and decision modelling.

In the area of **text and web mining, and heterogeneous information network analysis**, we successfully completed (with an excellent evaluation) the MULTIPLEX project (Foundational Research on MULTIllevel comPLEX networks and systems). We continued work on an existing FP7 project SIMPOL (Financial Systems Simulation and Policy Modelling) and a H2020 FET project DOLFINS (Distributed Global Financial Systems for Society). We also started a new national project FORMICA (Influence of formal and informal corporate communications on capital markets).

**The NAO robot talking through the WHIMBOT interface, developed within the WHIM project, attracted a lot of attention at this year's International fair of crafts and entrepreneurship in Celje.**

The main emphasis of the research in this area is combining text mining, network analysis and sentiment analysis to reveal and highlight

underlying properties in different domains. The main sources of data that we analyse are social media (Twitter, Facebook), online news, and other relevant data (e.g., voting in the European Parliament, stock prices, results of elections and referendums).

We collected tweets from the members of the European Parliament (EP), constructed retweet networks, and identified political and national communities. We also analysed the voting of the current, eighth EP, and compared the relation between the co-voting and retweeting. The results show that retweeting is very similar to co-voting, but also that the right-wing political groups are much more active and coherent in social media.

We developed methodology and tools to analyse Twitter sentiment (or stance) in different languages and for different topics. Our approach relies on a large set of manually annotated tweets by domain experts, and results in high-quality domain- and language-specific classification models. We showed how to estimate an upper bound of performance for a classification model and how to monitor the annotation process.

Finally, we applied the above-developed methodology to a highly relevant European use-case: the UK referendum on Brexit. We developed a Brexit-specific Twitter stance classification model and used it to monitor the public mood before and during the referendum. We also identified the most influential Twitter users and noted that the proponents of Brexit were considerably more active than the remain camp.

In the area of **decision support** our long-term goal is to develop methods and techniques of decision modelling, support them with software and integrate them with data-mining systems. In 2016 we published the results of applying these methods in two areas: assessment of long-term sustainability of electric energy production in Slovenia and assessment of potential presence of genetically modified crops in food and feed based on traceability data (Project DECATHLON). In each of these areas we developed a corresponding decision-support system. We also successfully used our qualitative multi-criteria modelling method DEX for the assessment of anthropogenic activities on the ecology of the Fifth Triglav Lake in the Julian Alps and for the evaluation of business process simulation software. We investigated and compared three methods for approximating incompletely defined utility functions with the DEX method. In the framework of the European project HeartMan we were developing decision models and systems for supporting patients having

Congestive Heart Failure. For the European project PD\_manager we have developed several decision-support models based on the expert knowledge of the clinical project partners, which reflect current knowledge in the Parkinson's disease domain regarding the medication changes, but had not been previously formalized. Regarding software



Figure 3: Winning team of the ESA's Mars Express Power Challenge visiting ESA Mission Control Centre (ESOC) in Darmstadt.

tools, in addition to updating the existing DEXi model-development program and JDEXi library, we developed the DEXi HTML Evaluator, a new software for the evaluation of decision alternatives using DEX models, which runs on web pages that require almost no programming to set up.

In the area of **language technologies and digital humanities** we work on producing language resources and methods to annotate text with linguistic information, with a focus on the Slovene language. In 2016 we helped to produce the digital text-critical edition of the 18th century Kapla passion play and worked on methods to modernise historical Slovene language, as well as standardising Slovene as found on the web. We have converted the ssj500k treebank into the Universal Dependencies framework and made the resulting treebank available in the scope of the UD project.

We continued work on the national research project JANES “Resources, Tools and Methods for Research of Non-standard Internet Slovene”, where we compiled the penultimate version of the JANES corpus of user-generated internet Slovene, which contains over 160 million words of tweets, news comments, forums, blogs and Wikipedia talk pages and researched ways in which to make such corpora openly available. We developed a method for restoring diacritics which are often missing in internet texts, developed a new part-of-speech tagger and lemmatiser, made our tools available as web applications, performed and analysed automatic sentiment labelling on internet texts, developed a method to detect semantic shifts in Slovene tweets, to distinguish private from corporate users, and performed analytics over them. We also studied the global use of emojis in tweets as well as sociolinguistic aspects, regarding the relation between the topic and gender of the user as well as the gender-representation on the web. We worked on the manual annotation of user-generated internet texts, concentrating on normalisation, part-of-speech tagging, lemmatisation and syntactic annotation with the motivation to produce training sets for machine-learning annotation tools for (non-standard) Slovene. We started work on a dictionary of Twitter-specific lexis and undertook several linguistic analyses on various aspects of user-generated internet texts, such as the use of the comma.

We started work on our new national research project KAS “Slovene scientific texts: resources and description”, where we produced the prototype version of the KAS corpus, which contains almost one billion words of scientific texts gathered from the digital libraries of Slovene universities and, on the basis of this corpus, performed an analysis on the use of the passive in Slovene scientific writing. As preparation on terminology extraction, we constructed a term grammar for the Sketch Engine corpus analysis platform.

In the scope of the industrial project TermIolar with the Slovene translation company Iolar, we developed a system for terminology management, integrating automatic terminology extraction from translation memories and existing terminological databases.

We lead the Slovene research infrastructure CLARIN.SI, which provides easy publication and sustainable access to digital language data for scholars in the humanities and social sciences. In 2016 the CLARIN.SI repository for language resources and tools was recognised as a CLARIN Center B, certifying it as a stable and trusted repository that conforms to the CLARIN technical and organisational standards. In this year the number of deposited resources in the repository more than doubled, reaching 47 at the end of the year, with the most interesting additions being a transcribed speech corpus of Slovene public lectures and a corpus of parliamentary debates from the years 1990–1992. In 2016 CLARIN.SI has also organised the international workshop “Multilingual corpus annotation tools: development and integration” and supported several conferences and summer schools.

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. We also continue to serve as technical editors for the on-line Slovene Biographic Lexicon.

In 2016 we organised the 10th biennial conference on Language Technologies, which was this year extended with the theme of Digital Humanities. The conference, which took place at the Arts Faculty of the University of Ljubljana, lasted three days with parallel sessions, and comprised five invited lectures, a round table on terminology, a student session, and 47 regular contributions.

In the field of **computational creativity** we continued to develop new prototype solutions using our tool ConCreTeFlows, which is based on our platform CloudFlows. Within the FP7 project CONCRETE (Concept Creation Technologies) we prepared a workflow for the multimodal mixing of concepts, which also served for the demonstra-

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**Vid Podpečan received the Prometheus of Science award for excellence in communication for the year 2016 from the Slovenian Science Foundation.**

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*Figure 4: Our NAO WHIMBOT attracted a lot of attention at the International fair of crafts and entrepreneurship in Celje.*

tion of ConCreTeFlows and its ability to support teamwork and the use of a variety of program elements in a single workflow. Presentation of the system with this demonstration at the International Conference on Computational Creativity ICCC 2016 was met with a positive response from the research community. We analysed the role of optimality principles in different conceptual blending systems and proposed the conceptualization of computational creativity. Within FP7 project WHIM (The What-If Machine) we conducted the final experiments of human

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**Sašo Džeroski was elected to the European Academy of Sciences (Academia Europaea).**

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appreciation modelling of computer generated what-if ideas and presented the system for scientific question generation. This year, the project WHIM achieved a remarkable achievement for the computational creativity research community: on the basis of computer-generated ideas from the WHIM system and other computational creativity approaches, a musical was made and presented on stage in London. In relation to that, a documentary was filmed about this venture and the technologies that were used to achieve it. In 2016, the projects of FP7: Prosecco, WHIM (The What-If Machine) and ConCreTe (Concept Creation Technologies) were finished and the results of the projects, as well as the wider area of computational creativity, were presented at invited talk of the TTT conference TTT 2016.

### Some outstanding publications in the last year

1. Adhikari, P. R., Vavpetič, A., Kralj, J., Lavrač, N., Hollmén, J. Explaining mixture models through semantic pattern mining and banded matrix visualization. *Machine learning*, ISSN 0885-6125. 2016, 37 pp., doi: 10.1007/s10994-016-5550-3.
2. Bohanec, M., Mileva-Boshkoska, B., Prins, T. W., Kok, E. SIGMO: a decision support System for Identification of genetically modified food or feed products. *Food control*, ISSN 0956-7135. 2016, vol. 71, pp. 168-177, doi: 10.1016/j.foodcont.2016.06.032.
3. Bohanec, M., Trdin, N., Kontić, B. A qualitative multi-criteria modelling approach to the assessment of electric energy production technologies in Slovenia. *Central European Journal of Operations Research*, ISSN 1435-246X, 2016, 15 pp., doi: 10.1007/s10100-016-0457-4.
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7. Perovšek, M., Kranjc, J., Erjavec, T., Cestnik, B., Lavrač, N. TextFlows : a visual programming platform for text mining and natural language processing. *Science of computer programming*, ISSN 0167-6423, 2016, vol. 121, str. 128-152, doi: 10.1016/j.scico.2016.01.001.
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### Awards and appointments

1. Matej Petkovič was awarded the Prešeren Prize of the Faculty of Mathematics and Physics of the University of Ljubljana for his master's thesis titled "Evaluation of the importance of continuous features with the ReliefF method", written under the supervision of Sašo Džeroski.
2. Sašo Džeroski, corresponding member of the Macedonian Academy of Arts and Sciences, was elected for a full member of the European Academy of Sciences (Academia Europaea).
3. Vid Podpečan received the Prometheus of Science award for excellence in communication for the year 2016 from the Slovenian Science Foundation for the all-round promotion of robotics, especially humanoid robot use among young people.
4. Special recognition for successful cooperation with the Committee on Science and Technology of the Chamber of craft and small business of Slovenia and for an interesting presentation of the Department of Knowledge Technologies of the Jožef Stefan Institute at the International fair of crafts and entrepreneurship in Celje.

5. Martin Breskvar, Dragi Kocev, Jurica Levatić, Aljaž Osojnik, Matej Petković, Nikola Simidjievski and Bernard Ženko won the ESA's Mars Express Power Challenge, designing the most accurate solution for predicting the space probe's power consumption.

## Organization of conferences, congresses and meetings

1. Workshop CLARIN "Multilingual corpus annotation tools: development and integration", Ljubljana, 10.-11. 11. 2016
2. "Summer school on mining big and complex data", Ohrid, Macedonia, 4.-8. 9. 2016
3. Final meeting of EU project "Concept Creation Technology" - ConCreTe, Bled, 14.-16. 9. 2016.

## INTERNATIONAL PROJECTS

1. BIODIV - Understanding and Managing Biodiversity in Agricultural Ecosystems by Data Mining and Decision Support  
Prof. Sašo Džeroski  
Arvalis - Institut Du Végétal
2. 7FP - PROSECCO; Promoting the Scientific Exploration of Computational Creativity  
Prof. Nada Lavrač  
European Commission
3. 7FP - ConCreTe; Concept Creation Technology  
Prof. Nada Lavrač  
European Commission
4. 7FP - WHIM; The What-If Machine  
Prof. Nada Lavrač  
European Commission
5. 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
6. 7FP - SIMPOL; Financial Systems Simulation and Policy Modelling  
Prof. Igor Mozetič  
European Commission
7. 7FP - MULTIPLEX; Foundational Research on Multilevel Complex Networks and Systems  
Prof. Igor Mozetič  
European Commission
8. 7FP - HBP; The Human Brain Project  
Prof. Sašo Džeroski  
European Commission
9. 7FP - MAESTRA; Learning from Massive, Incompletely Annotated, and Structured Data  
Prof. Sašo Džeroski  
European Commission
10. PARSEME: PARsing and Multi-Word Expressions. Towards Linguistic Precision and Computational Efficiency in Natural Language Processing  
Prof. Tomaž Erjavec  
Cost Office
11. H2020 - DOLFINS; Distributed Global Financial Systems for Society  
Prof. Igor Mozetič  
European Commission
12. H2020 - HBP SGA1; Human Brain Project Specific Grant Agreement 1  
Prof. Sašo Džeroski  
European Commission
13. H2020 - PD\_manager; Mhealth Platform for Parkinson's Disease Management  
Dr. Dragana Miljković  
European Commission
14. H2020 - HeartMan; Personal Decision Support System for Heart Failure Management  
Prof. Marko Bohanec  
European Commission
15. Mining Complex Data in Environmental and Life Sciences  
Prof. Sašo Džeroski  
Slovenian Research Agency
16. Mining Heterogeneous Linked Biomedical Data  
Prof. Nada Lavrač  
Slovenian Research Agency
17. Semantic Role Labeling in Slovene and Croatian  
Prof. Tomaž Erjavec  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Knowledge Technologies  
Prof. Nada Lavrač

## R & D GRANTS AND CONTRACTS

1. Slovenian Literature in Unknown Early Modern Manuscripts: Information-Technology Aided Analyses and Scholarly Editions  
Prof. Tomaž Erjavec
2. Integrative research of sexual dimorphism evolution  
Prof. Sašo Džeroski
3. Resources, Tools and Methods for the Research of Nonstandard Internet Slovene  
Prof. Tomaž Erjavec
4. Slovene scientific texts: resources and description  
Prof. Tomaž Erjavec
5. Analysis of heterogeneous information networks for knowledge discovery in life-sciences  
Prof. Nada Lavrač
6. Molecular bases of interactions among the grapevine and phytoplasmal causing agents of the grapevine yellows diseases  
Prof. Nada Lavrač
7. Development of a multimethod approach to study wildlife behavior: investigating humanbear conflicts in contrasting landscapes of Europe  
Prof. Sašo Džeroski
8. Influence of formal and informal corporate communications on capital markets  
Dr. Senja Pollak
9. Development and applications of new semantic data mining methods in life sciences  
Prof. Nada Lavrač
10. Machine Learning for Systems Sciences  
Prof. Sašo Džeroski
11. Forbidden Books in the Slovenian Lands in the Early Modern Period  
Prof. Tomaž Erjavec
12. Structured output prediction with applications in sustainable agricultural production  
Prof. Sašo Džeroski
13. ReLDI - Regional Linguistic Data Initiative  
Dr. Nikola Ljubešić  
University Of Zurich, Urpp Language And Space
14. CLARIN Workshop: „Multilingual Corpus Annotation Development and Integration“, IJS, Ljubljana, Slovenia; 10.11.-11.11.2016  
Prof. Tomaž Erjavec  
Clarín Eric
15. Methods of digital ethnography and monitoring of experiences and the development of global competencies of Erasmus students  
Dr. Martin Žnidaršič  
CMEPIUS

## NEW CONTRACTS

1. Development of a Prototype program solution for support of semi-automatic extraction and management of monolingual and multilingual corpora  
Dr. Senja Pollak  
Iolar d. o. o.

## VISITORS FROM ABROAD

1. Dario Stojanovski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, Skopje, Macedonia, 18.1.-7.2. 2016
2. Dr. Gjorgji Strezoski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, Skopje, Macedonia, 18.1.-7.2. 2016
3. Dr. Gjorgji Madjarov, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, Skopje, Macedonia, 31.1.-7.2.2016
4. Dr. Ivica Dimitrovski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, Skopje, Macedonia, 31.1.-7.2.2016



5. Andreas Karpf, UPIP - Centre d'Economie de la Sorbonne, Université Paris, Paris, France, 20.2.-31.3.2016
6. Matej Mihelčič, Institut Ruder Bošković, Zagreb, Croatia, 3.3.2016
7. Matija Piškorec, Institut Ruder Bošković, Zagreb, Croatia, 3.3.2016
8. dr. Larisa Soldatova, Brunel University, London, Great Britain, 21. 3. 2016
9. prof. dr. Ross King, University of Manchester, Manchester, Great Britain, 21.3.2016
10. Fabiana Zollo, IMT, School for Advanced studies Lucca, Lucca, Italy, 9.4.-1.7.2016.
11. Amilcar Cardoso, Coimbra University, Coimbra, Portugal, 13.-15. 4. 2016
12. Ana Oliveira Alves, Coimbra University, Coimbra, Portugal, 13.-15. 4. 2016
13. João Carlos Gonçalves, Coimbra University, Coimbra, Portugal, 13.-15. 4. 2016
14. dr. Tomislav Šmuc, Institut Ruder Bošković, Zagreb, Croatia, 3.3.2016 and 9.-13. 5. 2016
15. prof. dr. Filip Železny, Department of Computer Science, Faculty of Electrical Engineering, Czech Technical University in Prague, Prague, Czech Republic, 8.-10. 5. 2016
16. Jožef Mišutka, Karlova univerza v Prazi, Prague, Czech Republic, 11.-16. 4. 2016
17. dr. Barry Hardy, Douglas Connect, Basel, Switzerland, 3.-6. 5. 2016
18. prof. dr. Ljupčo Kocarev, Macedonian Academy of Sciences and Arts, Skopje, Macedonia, 22.-24. 5. 2016
19. Ivan Stojković, Temple University, Philadelphia, USA, 20.-22.7.2016
20. Dr. Daniel Zeman, Karlova Univerza, Prague, Czech Republic, 28.9.-1. 10. 2016
21. dr. Petru Juelu Henrichsenu, Copenhagen Business School, Copenhagen, Denmark, 29. 9.- 1. 10. 2016
22. Filip Petkovski, Zagreb, Croatia, 26.-28.9.2016
23. Vera Veleva, BILSP, Bulgaria, 25. 10. 2016
24. Yordan Dimitrov, BILSP, Bulgaria, 25. 10. 2016
25. Ben Verhoeven, University of Antwerp, Antwerp, Belgium, 31. 10.-26. 11. 2016
26. prof. dr. Bogdan Draganski Centre hospitalier universitaire vaudois, Luzana, Switzerland, 13.-15. 11. 2016
27. dr. Florence Leprince, ARVALIS-Institut du végétal, Pau, France, 24.-25. 11. 2016
28. dr. Markus Schedl, Department of Computational Perception, Johannes Kepler University (JKU) Linz, Austria, 15. 12. 2016

## STAFF

### Researchers

1. Prof. Marko Bohanec
2. Prof. Bojan Cestnik\*
3. Prof. Marko Debeljak
4. Prof. Sašo Džeroski
5. Prof. Tomaž Erjavec
6. Dr. Darja Fišer\*
7. Dr. Dragi Kocev
8. **Prof. Nada Lavrač, Head**
9. Prof. Zoran Levnajič\*
10. Prof. Igor Mozetič
11. Prof. Ljupčo Todorovski\*
12. Prof. Tanja Urbančič\*
13. Asst. Prof. Martin Žnidaršič

### Postdoctoral associates

14. Dr. Darko Aleksovski
15. *Dr. Darko Čerepnalkoski, left 01.11.16*
16. Dr. Miha Grčar
17. Dr. Petra Kralj Novak
18. Dr. Nikola Ljubešič
19. Asst. Prof. Biljana Mileva Boshkoska
20. Dr. Dragana Miljković
21. Asst. Prof. Panče Panov
22. Dr. Vid Podpečan
23. Dr. Senja Pollak
24. Dr. Nikola Simidjievski

25. *Dr. Borut Sluban, left 01.10.16*

26. Dr. Jasmina Smailović
27. Dr. Jovan Tanevski
28. Dr. Aneta Trajanov
29. Dr. Anže Vavpetič
30. Dr. Vedrana Vidulin
31. Asst. Prof. Bernard Ženko

### Postgraduates

32. Martin Breskvar, B. Sc.
33. Jan Kralj, B. Sc.
34. Janez Kranjc, B. Sc.
35. Jurica Levatič
36. Aljaž Osojnik
37. *Dr. Matic Peroušek, left 01.07.16*
38. Matej Petković, B. Sc.
39. Tomaž Stepišnik Perdih, B. Sc.
40. Anita Valmarska, B. Sc.
41. Katja Zupan, B. Sc.

### Technical officers

42. Tina Anžič, B. Sc.
43. Milica Bauer, B. Sc.

### Technical and administrative staff

44. *Teja Dukič, 01.10.16, transferred to Department K7*

Note:

\* part-time JSI member

# BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Prem Raj Adhikari, Anže Vavpetič, Jan Kralj, Nada Lavrač, Jaakko Hollmén, "Explaining mixture models through semantic pattern mining and banded matrix visualization", *Mach. learn.*, vol. 105, iss. 1, pp. 3-39, 2016.
2. Darko Aleksovski, Juš Kocijan, Sašo Džeroski, "Ensembles of fuzzy linear model trees for the identification of multi-output systems", *IEEE trans. fuzzy syst.*, vol. 24, no. 4, pp. 916-929, 2016.
3. Marko Bohanec, Biljana Mileva-Boshkoska, Theo W. Prins, Esther Kok, "SIGMO: a decision support System for Identification of genetically modified food or feed products", *Food control*, vol. 71, pp. 168-177, 2016.
4. Marija Brbič, Matija Piškorec, Vedrana Vidulin, Anita Kriško, Tomislav Šmuc, Fran Supek, "The landscape of microbial phenotypic traits and associated genes", *Nucleic acids res.*, vol. 44, no. 21, pp. 10074-10090, 2106.
5. Darko Čerepnalkoski, Andreas Karpf, Igor Mozetič, Miha Grčar, "Cohesion and coalition formation in the European parliament: roll-call votes and twitter activities", *PLoS one*, vol. 11, no. 11, pp. 0166586-1-0166586-27, 2016.
6. Darko Čerepnalkoski, Igor Mozetič, "Retweet networks of the European Parliament: evaluation of the community structure", *Appl. netw. sci.*, vol. 1, no. 1, pp. 2-1-2-20, 2016.
7. Nadja Damij, Pavle Boškoski, Marko Bohanec, Biljana Mileva-Boshkoska, "Ranking of business process simulation software tools with DEX/QQ hierarchical decision model", *PLoS one*, vol. 11, no. 2, pp. 0148391-1-0148391-16, 2016.
8. Ivica Dimitrovski, Dragi Kocev, Suzana Loskovska, Sašo Džeroski, "Improving bag-of-visual-words image retrieval with predictive clustering trees", *Inf. sci.*, vol. 329, pp. 851-865, 2016.
9. Tomaž Erjavec, Jaka Čibej, Darja Fišer, "Omogočanje dostopa do korpusov slovenskih spletnih besedil v luči pravnih omejitev", In: *Računalniško posredovana komunikacija*, (Slovenščina 2.0, Tematska številka, vol. 4 (2016), no. 2), Darja Fišer, ed., Ljubljana, Trojina, zavod za uporabno slovenistiko, 2016, vol. 4, no. 2, pp. 189-219, 2016.
10. Darja Fišer, Tomaž Erjavec, Nikola Ljubešič, "JANES v0.4: korpus slovenskih spletnih uporabniških vsebin", In: *Računalniško posredovana komunikacija*, (Slovenščina 2.0, Tematska številka, vol. 4 (2016), no. 2), Darja Fišer, ed., Ljubljana, Trojina, zavod za uporabno slovenistiko, 2016, vol. 4, no. 2, pp. 67-99, 2016.
11. Dragan Gamberger, Bernard Ženko, Alexis Mitelpunkt, Netta Shchar, Nada Lavrač, "Clusters of male and female Alzheimer's disease patients in the Alzheimer's Disease Neuroimaging Initiative (ADNI) database", *Brain inform.*, vol. 3, iss. 3, pp. 169-179, 2016.
12. Sašo Jančič, Jens C. Frisvald, Dragi Kocev, Cene Gostinčar, Sašo Džeroski, Nina Gunde-Cimerman, "Production of secondary metabolites in extreme environments: food- and airborne *Walleria* spp. produce toxic

- metabolites at hypersaline conditions", *PLoS one*, vol. 11, no. 12, pp. e0169116-1-e0169116-20, 2016.
13. Sašo Jančič, Polona Zalar, Dragi Kocev, Hans-Josef Schroers, Sašo Džeroski, Nina Gunde-Cimerman, "Halophily reloaded: new insights into the extremophilic life-style of *Walleimia* with the description of *Walleimia hederæ* sp. nov.", *Fungal divers.*, vol. 76, issue 1, pp. 97-118, 2016.
  14. Branko Kontič, Marko Bohanec, Davor Kontič, Nejc Trdin, Maruša Matko, "Improving appraisal of sustainability of energy options - a view from Slovenia", *Energy policy*, vol. 90, pp. 154-171, 2016.
  15. Zoran Krstanoski, Nadja Kokalj-Vokač, Andreja Zagorac, Boris Pospihalj, Miha Munda, Sašo Džeroski, Rastko Golouh, "TMRSS2:ERG gene aberrations may provide insight into pT stage in prostate cancer", *BMC Urol*, vol. 16, pp. 1-6, 2016.
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  17. Gjorgji Madjarov, Dejan Gjorgjevič, Ivica Dimitrovski, Sašo Džeroski, "The use of data-derived label hierarchies in multi-label classification", *Journal of intelligent information systems*, vol. 47, iss. 1, pp. 57-90, 2016.
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  19. Igor Mozetič, Miha Grčar, Jasmina Smailović, "Multilingual twitter sentiment classification: the role of human annotators", *PLoS one*, vol. 11, no. 5, pp. e0155036-1-e0155036-26, 2016.
  20. Monika Novak, Polona Zalar, Bernard Ženko, Sašo Džeroski, Nina Gunde-Cimerman, "Yeasts and yeast-like fungi in tap water and groundwater, and their transmission to household appliances", *Fungal ecology*, vol. 20, pp. 30-39, 2016.
  21. Aljaž Osojnik, Panče Panov, Sašo Džeroski, "Modeling dynamical systems with data stream mining", *Comput. Sci. Inf. Syst.*, vol. 13, no. 2, pp. 453-473, 2016.
  22. Panče Panov, Larisa N. Soldatova, Sašo Džeroski, "Generic ontology of datatypes", *Inf. sci.*, vol. 329, pp. 900-920, 2016.
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  24. Tina Ravnikar, Marko Bohanec, Gregor Muri, "Monitoring and assessment of anthropogenic activities in mountain lakes: a case of the Fifth Triglav Lake in the Julian Alps", *Environ. monit. assess.*, vol. 188, pp. 253-1-253-17, mar. 2016.
  25. Yves Scherrer, Tomaž Erjavec, "Modernising historical Slovene words", *Nat. lang. eng.*, vol. 22, no. 6, pp. 881-905, 2016.
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  27. Ana Marija Sobočan, Senja Pollak, "Manifestacije moralne panike v medijskih podobah novele družinske zakonodaje", *Čas. krit. znan.*, vol. 44, no. 266, pp. 163-187, 2016.
  28. Darja Šemrov, Rok Marsetič, Marijan Žura, Ljupčo Todorovski, Aleksander Srdič, "Reinforcement learning approach for train rescheduling on a single-track railway", *Transp. res., Part B: methodol.*, vol. 86, no. apr., pp. 250-267, 2016.
  29. Bosiljka Tadić, Miroslav Andjelković, Biljana Mileva-Boshkoska, Zoran Levnajić, "Algebraic topology of multi-brain connectivity networks reveals dissimilarity in functional patterns during spoken communications", *PLoS one*, vol. 11, no. 11, pp. e0166787-1-e0166787-25, 2016.
  30. Jovan Tanevski, Ljupčo Todorovski, Sašo Džeroski, "Learning stochastic process-based models of dynamical systems from knowledge and data", *BMC systems biology*, vol. 10, pp. 30-1-30-17, 2016.
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  32. Vedrana Vidulin, Tomislav Šmuc, Fran Supek, "Extensive complementarity between gene function prediction methods", *Bioinformatics (Oxf.)*, vol. 32, no. 23, pp. 3645-3653, 2016.
  33. *Proceedings of the 4th IFAC Conference on Intelligent Control and Automation, ICONS 2016, 1-3 June 2016, Reims, France*, (IFAC papersOnline, Vol. 49, no. 5, 2016), pp. 31-36.
  34. Špela Arhar Holdt, Darja Fišer, Tomaž Erjavec, Simon Krek, "Syntactic annotation of Slovene CMC: first steps", In: *Proceedings of the 4th Conference on CMC and Social Media Corpora for the Humanities, 27-28 September 2016, Faculty of Arts, University of Ljubljana, Ljubljana, Slovenia*, pp. 3-6.
  35. Renato Barišič, Biljana Mileva-Boshkoska, "MIMOSA OSA-EAI: an information exchange standard: standard razmjene informacija", In: *Kvaliteta čini razliku: zbornik radova: proceedings*, pp. 45-57.
  36. Michael Beißwenger et al. (12 authors), "Integrating corpora of computer-mediated communication into the language resources landscape: initiatives and best practices from French, German, Italian and Slovenian projects", In: *Proceedings*, pp. 1-5.
  37. Jože Bučar, Janez Povh, Martin Žnidaršič, "Sentiment classification of the Slovenian news texts", In: *Proceedings of the 9th International Conference on Computer Recognition Systems CORES 2015*, (Advances in intelligent systems and computing, Vol. 403, 2016), pp. 777-787.
  38. Bojan Cestnik, Elsa Fabbretti, Donatella Gubiani, Nada Lavrač, Tanja Urbančič, "Exploring outlier documents to investigate potential links between gut microbiota and Alzheimer's disease", In: *Proceedings, extended abstracts, IWBBIO 2016, International Work-Conference on Bioinformatics and Biomedical Engineering, April 20-22, 2016, Granada, Spain*, pp. 475-486.
  39. Bojan Cestnik, Natalia Manakova, Aram Karalič, Tanja Urbančič, "Engaging the net generation students in enhanced teaching and learning with QTvity: the next steps", In: *Proceedings: European thematic network, future education and training in computing: how to support learning at anytime anywhere*, International Conference on e-Learning, 8-9 September, Bratislava, Slovakia, pp. 86-93.
  40. Jaka Čibej, Špela Arhar Holdt, Tomaž Erjavec, Darja Fišer, "Razvoj učne množice za izboljšano označevanje spletnih besedil", In: *Zbornik konference Jezikovne tehnologije in digitalna humanistika, 29. september - 1. oktober 2016, Filozofska fakulteta, Univerza v Ljubljani, Ljubljana, Slovenija*, pp. 40-46.
  41. Jaka Čibej, Darja Fišer, Tomaž Erjavec, "Normalisation, tokenisation and sentence segmentation of Slovene tweets", In: *Normalisation and analysis of social media texts (NormSoMe): [workshop proceedings]*, pp. 5-10.
  42. Marko Debeljak, Andrej Ficko, Robert Brus, "Ocena ogroženosti avtohtonih drevesnih vrst pred invazivnimi tujerodnimi vrstami na primeru črnega topola (*Populus nigra* L.): the case of Black poplar (*Populus nigra* L.)", In: *Invazivne tujerodne vrste v gozdovih ter njihov vpliv na trajnostno rabo gozdnih virov: zbornik prispevkov posvetovanja z mednarodno udeležbo: lectures presented at the conference with international participation*, 2016, pp. 119-124.
  43. Tomaž Erjavec, Špela Arhar Holdt, Jaka Čibej, Kaja Dobrovoljc, Darja Fišer, Cyprian Laskowski, Katja Zupan, "Annotating CLARIN.SI TEI corpora with WebAnno", In: *Proceedings*, 2016, pp. 1-5.
  44. Tomaž Erjavec, Jaka Čibej, Špela Arhar Holdt, Nikola Ljubešič, Darja Fišer, "Gold-standard datasets for annotation of Slovene computer-mediated communication", In: *RASLAN 2016: Recent Advances in Slavonic Natural Language Processing: proceedings*, pp. 29-40.
  45. Tomaž Erjavec, Darja Fišer, Nikola Ljubešič, Nataša Logar, Milan Ojsteršek, "Slovenska znanstvena besedila: prototipni korpus in načrt analiz", In: *Zbornik konference Jezikovne tehnologije in digitalna humanistika, 29. september - 1. oktober 2016, Filozofska fakulteta, Univerza v Ljubljani, Ljubljana, Slovenija*, pp. 58-64.
  46. Darja Fišer, Tomaž Erjavec, "Analysis of sentiment labeling of Slovene user-generated content", In: *Proceedings of the 4th Conference on CMC and Social Media Corpora for the Humanities, 27-28 September 2016, Faculty of Arts, University of Ljubljana, Ljubljana, Slovenia*, pp. 22-25.
  47. Darja Fišer, Nikola Ljubešič, "Detecting semantic shifts in Slovene twitterese", In: *RASLAN 2016: Recent Advances in Slavonic Natural Language Processing: proceedings*, pp. 43-50.
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  49. Darja Fišer, Vit Suchomel, Miloš Jakubiček, "Terminology extraction for academic Slovene using sketch engine", In: *RASLAN 2016: Recent Advances in Slavonic Natural Language Processing: proceedings*, pp. 135-141.
  50. Dragan Gamberger, Bernard Ženko, Alexis Mitelpunkt, Nada Lavrač, "Homogeneous clusters of Alzheimer's disease patient population", In: *Selected articles of the 3rd International Work-Conference on*

## PUBLISHED CONFERENCE CONTRIBUTION

1. Darko Aleksovski, Dejan Dovžan, Sašo Džeroski, Juš Kocijan, "A comparison of fuzzy identification methods on benchmark datasets", In:

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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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, language and speech technologies, and smart cities together with electronic and mobile health. The department collaborates closely with the Faculty of Computer and Information Science of the University of Ljubljana on the joint research program “Artificial Intelligence and Intelligent Systems”, led by Prof. Dr. Ivan Bratko. The department also closely collaborates with industry and significantly contributes the introduction of intelligent systems into products and services.*



Head:  
**Prof. Matjaž Gams**

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, while they also exploit raw, exponentially growing computer power. This field is somewhat broader than only artificial intelligence, both are rapidly improving worldwide and enabling the development of information society.

**Ambient intelligence** is a research area aiming to introduce technology into our everyday environment in a friendly way undemanding for the user. The main topic of ambient intelligence tackled by the department in 2016 was e-health. We started the H2020 project **HeartMan**, which we also coordinate. The project is developing an application that will help congestive-heart-failure patients manage their condition: it will monitor them with a sensing wristband, and provide advice on exercise, nutrition etc. So far we have developed decision models based on medical guidelines and user requirements, which will serve as the foundation for the application. Related to this project is the development of methods for the prediction of hospitalizations of heart-failure patients, and for the evaluation of their health based on stethoscope sound recordings. In the H2020 project **IN LIFE**, we are attempting to translate some solutions intended to prolong the independence of the elderly into real life. We prepared a smart-watch application that detects falls and similar events. This application is connected to a web application through which the carers can monitor their charges, send them messages and organize home visits. By the end of the year this solution was sufficiently mature to be used in pilots with 150 users, to be organized in cooperation with the Slovenian company Doktor 24 in early 2017. The AAL project **Fit4Work** is aiming to help older workers do their job more easily by providing advice on relaxation, exercise and work environment (temperature, CO<sub>2</sub> in the air etc.). To this end, we developed a method that recognizes mental stress using a wristband with physiological sensors. The method takes into account the context of a potentially stressful event, which makes it highly accurate. We also developed a method that can analyze physical activity with the sensors in the wristband and smartphone regardless of which device is worn and where. Finally, we use an ontology to select reasonable actions to improve the work environment, after which we simulate the outcome of each and recommend the best one. All our ambient-intelligence projects use wearable sensing devices, whose use is limited by their typically small batteries. As **doctoral research**, we are therefore developing a general method that can intelligently turn sensors on and off in such a way that the energy consumption is as small as possibly without sacrificing a lot of quality of the results obtained with these sensors.

**Computational intelligence** is a study of stochastic search, optimization and learning methods, inspired by biological and physical systems. Research in this area at the Department of Intelligent Systems focuses on

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**In the IN LIFE project we developed a smart watch for the elderly and we are running pilot tests on 150 users.**

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*Figure 1: Within the framework of the H2020 IN LIFE project we developed a smart watch for the elderly and prepared 150 pieces for a 6-month-long pilot testing. The watch allows around 10 functions, including calls to the carer, automatic fall detection, location identification and call for help, notifications, monitoring of physical activity, etc. The system is a personal assistant and carer for the elderly. Our vision is to introduce it to the care of the elderly Europe-wide, thus increasing the quality of life.*

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**In the AAL project Fit4Work we developed a method for stress detection using a wristband with physiological sensors. The method takes into account the context of a potentially stressful event, which makes it highly accurate.**

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**The embedded computer system for manufacturing quality control developed by the Jožef Stefan Institute and Kolektor Group company is a key achievement of the COPCAMS project.**

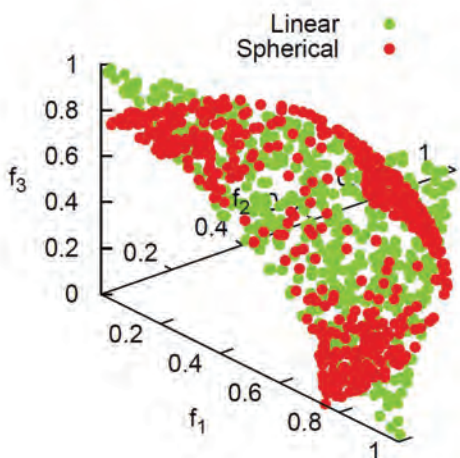


Figure 2: We design visualization methods for multiobjective optimization that assist decision-makers in selecting among trade-off solutions. A series of publications in the previous years was complemented with a tutorial given at the Genetic and Evolutionary Computation Conference (GECCO) 2016.

**The ACCUS project developed a coordination platform for smart cities that enables the control of various city subsystems and provides several services for citizens.**



Figure 3: A manufacturing quality control system resulting from the COPCAMS project is based on machine vision, machine learning and optimization.

**In the Smart Specialisation programs we are developing several solutions for smart cities and communities, smart building and homes, and sustainable food.**

the evolutionary computation methods. We study evolutionary algorithms for multiobjective optimization, their acceleration through parallel computing and surrogate models, visualization of their results, and applications in engineering design and optimization problems. These methods are being transferred to practice, especially in the area of production process optimization. In 2016, we finished the COPCAMS project approved for funding under the Artemis call. Together with the Slovene industrial partner

Kolektor Group and international partners, we developed a procedure for product quality control that is based on machine vision, machine learning and optimization, and operates on an embedded computer architecture. The procedure is now used in manufacturing of graphite commutators for automotive industry in Kolektor. It supports dimensional measurements, assessment of the cooper-graphite joints and non-contact measurements of commutator roughness. According to project reviewers, this was the most successful project achievement. We also started an H2020 Twinning project SYNERGY whose objective is to strengthen our research and innovation potential in parallelization and surrogate modelling and to explore the potential of combining the two techniques in multi-objective optimization. Three partners with complementary expertise cooperate in this endeavor: the Jožef Stefan Institute, the University of Lille, and Cologne University of Applied Sciences. The expertise and solutions gained through this cooperation will be disseminated to both academic and industrial organizations, particularly those participating in the Slovene Smart Specialisation Strategy. In addition, a bilateral Slovenian-Japanese research project was approved for funding and initiated. It is aimed at advancing the methodology of evolutionary multiobjective optimization for real-world applications. We cooperate with Shinshu University, Nagano, on developing optimization algorithms for space exploration and transportation network design.

In the field of agent and multi-agent systems the key research areas are focused on the development of smart autonomous systems for the control of smart cities, smart homes and the preservation of cultural heritage. In this year we have successfully concluded the European project ACCUS that aimed at developing an integration and coordination platform for urban systems to build applications across various domains, providing adaptive and cooperative control for urban subsystems, and optimizing the combined performance of the city. In the final presentation we presented a system for balancing the overall electricity consumption in the city by curbing the electricity spikes that occur during the day. In addition, the system optimizes the electricity consumption in smart houses and the production in thermal power plants, and manages the traffic flow and thus affects the external parameters, such as air quality. We continue the research in this area in the Smart Specialisation program EkoSMART in the field of smart cities and communities. The purpose of the program is to develop a smart city ecosystem with all the support mechanisms that are necessary for efficient, optimized and gradual integration of different smart city areas into a unified and well connected system. Within the program we are involved in activities linked to the research and development projects "Zasnova ekosistema pametnega mesta" and "Elektronsko in mobilno zdravstvo" (EMZ), where we are the lead partner. We are also involved in the Smart Specialisation program IQDOM in the field of smart buildings and homes, coordinated by Gorenje. Our focus will be 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 will apply similar learning algorithms also to 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, lowers the temperature of the stored water during days of lower consumption. In the Interreg AS-IT-IC project we will develop an integrated touristic platform for cross-border tourist exchange, tour planning and effective communication between tourists and tourist offices. In the

Horizon 2020 Twinning project **eHeritage** we continue to provide support to increase the capacity and quality of the research and innovation excellence of the Romanian partner in the area of cultural heritage preservation using intelligent methods and 3D modelling, and employing augmented and virtual reality. To this end, we organized the eHeritage workshop within the Information Society 2016 multiconference. During the same event the project partners presented products and applications based on the virtual reality technology (Heritage awareness day).

In the field of **speech and language technologies** we work on speech synthesis, semantic analysis of text and question answering. Together with companies Alpineon and Amebis we developed a new, high-quality speech synthesizer eBralec (<http://ebralec.si/>). The synthesizer is improved on both understandability and natural perception of the speech. The software package already has more than a thousand subscribers and is an indispensable tool of blind and visually-impaired users (it is the »official« speech synthesizer for the Society of visually impaired of Slovenia) and people with reading impairments (society Bravo). For these users, eBralec is free of charge and can be ordered in the Library for the blind and visually impaired (<http://www.kss-ess.si/ebralec-sintetizator-govora-slovenskega-jezika/>). Since 2016, the application DarsTraffic+, which provides users traffic information, also uses the eBralec software. This application was 1<sup>st</sup> on the App Store and 3<sup>rd</sup> in Google Play. According to the media, its key functionality and advantage are the audio settings. We have also developed the free service of speech synthesis for mobile devices (<http://dis.ijs.si/dyslex/>).

In collaboration with the Computer Systems Department, we organized the **7th International Conference on Bioinspired Optimization Methods and their Applications – BIOMA 2016** that took place from 18 to 20 May 2016 in Bled, Slovenia. The conference was devoted to theoretical and practical aspects of computer optimization methods inspired by natural phenomena. Its program consisted of 19 presentations by 45 coauthors from 11 countries. The invited lecturers were Prof. Thomas Bartz-Beielstein from the Cologne University of Applied Sciences and Prof. El-Ghazali Talbi from the University of Lille. Selected papers from the conference will be published in the extended form in the Applied Soft Computing journal. Collocated events were the 28th Slovene Workshop on Nature-Inspired Algorithms and the H2020 SYNERGY project meeting and training.

From 10 to 14 October 2015, the **19th International Multiconference Information Society – IS 2015** (is.ijs.si) took place at Jožef Stefan Institute. It consisted of 13 independent conferences with 200 presented papers. Four conference awards were presented: for lifetime achievements ("Donald Michie and Alan Turing" award) to Prof. Tomaž Pisanski, for current achievements in the field of information society to Prof. Blaž Zupan, and the information strawberry and lemon for the best and worst public information-society services.

### Some outstanding publications in the past year

1. Cvetkovič, B., Janko, V., Romero, A. E., Kafali, Ö., Stathis, K., Luštrek, M. Activity recognition for diabetic patients using a smartphone. *J. med. syst.*, 40 (2016) 256-1-256-8
2. Gjoreski, M., Gjoreski, H., Luštrek, M., Gams, M. How accurately can your wrist device recognize daily activities and detect falls?. *Sensors*, 16 (2016) 800-1-800-21
3. Tavčar, A., Kužnar, D., Gams, M. Hybrid multi-agent strategy discovering algorithm for human behavior. *Expert systems with applications*, 71 (2017) 370-382
4. Veček, N., Mernik, M., Filipič, B., Črepinšek, M. Parameter tuning with Chess Rating System (CRS-Tuning) for meta-heuristic algorithms. *Information Sciences*, 372 (2016), 446-469

### Organization of conferences, congresses and meetings

1. 28th Slovene Workshop on Nature-Inspired Algorithms, AVN, Bled, 18. 5. 2016
2. 7th International Conference on Bioinspired Optimization Methods and their Applications, BIOMA 2016, Bled, 18.-20. 5. 2016
3. Conference Genetic and Evolutionary Computation Conference, GECCO 2016, Denver, USA, 20.-24. 7. 2016



Figure 4: Fit4Work application, which helps older workers relax, be physically fit and have a good work environment (left). Measurements of human energy expenditure needed to develop the application (right).

**Together with companies Amebis and Alpineon, we developed a high-quality speech synthesizer eBralec (<http://ebralec.si/>).**

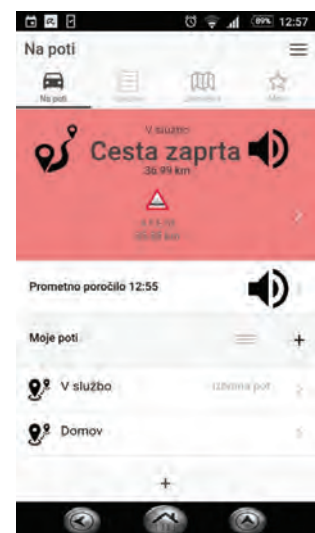


Figure 6: The application DarsTraffic+, which safely provides users traffic information, uses the eBralec software.

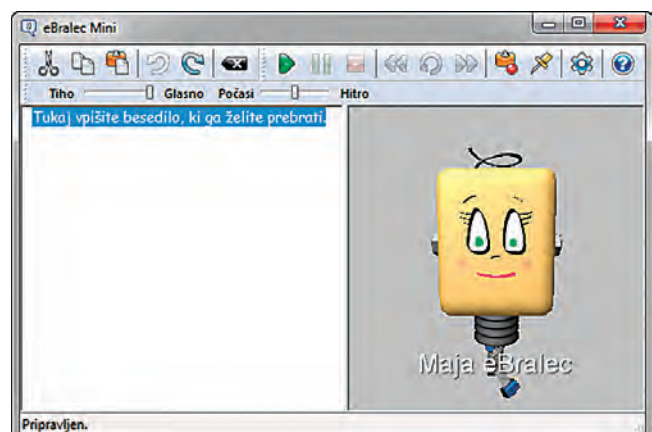


Figure 5: A new, high-quality speech synthesizer eBralec (<http://ebralec.si/>).



4. Workshop BBOB (Bi-Objective Blackbox Optimization Benchmarking) at Genetic and Evolutionary Computation Conference, GECCO 2016, Denver, USA, 20. 7. 2016
5. Workshop Women@GECCO at conference Genetic and Evolutionary Computation Conference, GECCO 2016, Denver, USA, 21. 7. 2016
6. Special Section Multiobjective Optimization with Surrogate Models, IEEE World Congress on Computational Intelligence, IEEE WCCI 2016, Vancouver, Canada, 24.-29. 7. 2016
7. Workshop Austrian-Slovenian Intelligent Tourist Information Center (AS-IT-IC), Ljubljana, Slovenia, 26. 9. 2016.
8. 19th International Multiconference Information Society, IS 2016, Ljubljana, Slovenia, 10.-14. 10. 2016; independent conferences:
  - Slovenian conference on artificial intelligence
  - Facing demographic challenges
  - Cognitive science
  - Collaboration, software and services in information society
  - Data mining and data warehouses
  - Human-computer interaction in information society (HCI-IS)
  - Workshop E-Heritage
  - Computer science and informatics: yesterday for tomorrow
  - 25th anniversary of internet in Slovenia
  - 3rd student computer science research conference
  - Ekosmart in EMZ
  - Education in information society (VIVID)
  - Middle-European conference on applied theoretical computer science (Matcos 2016)
9. eHeritage awareness day: presentation of virtual reality applications, Ljubljana, 13. 10. 2016
10. NATO Lecture series SET-235, Ljubljana, 27.-28. 10. 2016

### Patent granted

1. Matjaž Gams, Hristijan Gjoreski, Mitja Luštrek, Method and system for detecting a person driving a vehicle while using a mobile computing device, SI24796 (A), Slovenian Intellectual Property Office, 29. 02. 2016.

## INTERNATIONAL PROJECTS

1. Adaptive Cooperative Control in Urban (sub) Systems  
Prof. Matjaž Gams  
Ministrstvo za Gospodarstvo
2. COgnitive & Perceptive CAMeraS: COPCAMS  
Prof. Bogdan Filipič  
Ministrstvo za Gospodarstvo
3. Austrian-Slovenian Intelligent Tourist Information Center (AS-IT-IC)  
Prof. Matjaž Gams  
Služba Vlade Republike Slovenije za Razvoj
4. COST TD1405; ENJECT, European Network for the Joint Evaluation of Connected Health Technologies  
Božidara Cvetković, B. Sc.  
Cost Office
5. H2020 - IN LIFE; INdependent Living support Functions for the Elderly  
Prof. Matjaž Gams  
European Commission
6. H2020 - eHERITAGE; Expanding the Research and Innovation Capacity in Cultural Heritage Virtual Reality Applications  
Prof. Matjaž Gams  
European Commission
7. H2020 - HeartMan; Personal Decison Support System for Heart Failure Management  
Dr. Mitja Luštrek  
European Commission
8. H2020 - SYNERGY; Synergy for Smart Multi-Objective Optimisation  
Prof. Bogdan Filipič  
European Commission
9. Advanced Methodology of Evolutionary Multi- and Many-Objective Optimization for Real-World Applications  
Prof. Bogdan Filipič  
Slovenian Research Agency

## RESEARCH PROGRAM

1. Artificial Intelligence and Intelligent Systems  
Prof. Matjaž Gams

## R & D GRANTS AND CONTRACTS

1. Adaptive Cooperative Control in Urban (sub) Systems  
Prof. Matjaž Gams  
COgnitive & Perceptive CAMeraS: COPCAMS  
Prof. Bogdan Filipič  
Ministry of Economic of the Republic of Slovenia  
Self-management of physical and mental fitness of older workers  
Dr. Mitja Luštrek  
Ministry of Education, Science and Sport of the Republic of Slovenia
2. Conference BIOMA 2016; The 7th International Conference on Bioinspired Methods and their Applications, Bled, Slovenia, 18.-20.05.2016  
Prof. Bogdan Filipič
3. The 19th International Multiconference Information Society 2016 (IS2016), JSI, Ljubljana, Slovenia, 10 October - 14 October 2016  
Prof. Matjaž Gams
4. Intelligent home of the new generation designed on smart appliances and wood  
Prof. Matjaž Gams  
Ministry of Education, Science and Sport of the Republic of Slovenia
5. Smart City Ecosystem - EkoSmart  
Prof. Matjaž Gams  
Ministry of Education, Science and Sport of the Republic of Slovenia

## NEW CONTRACT

1. The inclusion of off-line speech synthesizer into the eBralec Mobile app for the Android operating system  
Dr. Tomaž Šef  
Amebis, d. o. o., Kamnik

## VISITORS FROM ABROAD

1. Boris Naujoks, Jörg Stork, Cologne University of Applied Sciences (TH Köln), Gummersbach, Germany, 10.-11. 2. 2016
2. El-Ghazali Talbi, prof. dr. Nouredine Melab, University Lille 1, Lille, France, 10.-11. 2. 2016
3. dr. Christian Fabre, dr. Alexandre Guerre, Julie Foucault, Commissariat à l'énergie atomique et aux énergies alternatives (CEA), Grenoble, France, 18. 4. 2016
4. Kenzi Djouhri, IUT de Cachan IUT de Cachan Génie Electrique, Paris, France, 25. 4.-15. 7. 2016
5. Thomas Justice, IUT de Cachan IUT de Cachan Génie Electrique, Paris, France, 25. 4.-15. 7. 2016
6. Hakim Kebli, IUT de Cachan IUT de Cachan Génie Electrique, Paris, France, 3. 5.-15. 7. 2016
7. Thomas Bartz-Beielstein, Jörg Stork, Martin Zaefferer, Cologne University of Applied Sciences (TH Köln), Gummersbach, Germany, 17. 5. 2016
8. Adam Benjelloun, IUT de Cachan, IUT de Cachan Génie Electrique, Paris, France, 20. 5.-12. 8. 2016
9. Timothée Foulon, IUT de Cachan, IUT de Cachan Génie Electrique, Paris, France, 20. 5.-12. 8. 2016
10. Florian Lemaître, IUT de Cachan IUT de Cachan Génie Electrique, Paris, France, 20. 5.-12. 8. 2016
11. prof. dr. Kiyoshi Tanaka, prof. dr. Hernán Aguirre, Shinshu University, Nagano, Japan, 23.-24. 5. 2016
12. Marzhan Kulbulatova, Kazakh-British Technical University, Almaty, Kazakhstan, 6. 6.-12. 8. 2016
13. Martin Bonchanoski, Faculty of Computer Science and Engineering, Ss Cyril and Methodius University, Skopje, Republic of Macedonia, 10. 9.-14. 10. 2016
14. prof. Csaba Antonya, Faculty of Mechanical Engineering, Transylvania University of Brasov, Brasov, Romania, 25. 9.-16. 10. 2016
15. dr. Eng. Eugen Valentin Butilă, Faculty of Technological Engineering, Transylvania University of Brasov, Brasov, Romania, 25. 9.-16. 10. 2016
16. Monika Simjanoska, Faculty of Computer Science and Engineering, Ss Cyril and Methodius University, Skopje, Republic of Macedonia, 24. 10.-30. 12. 2016
17. Boris Naujoks, Cologne University of Applied Sciences (TH Köln), Gummersbach, Germany, 10.-11. 11. 2016

## STAFF

### Researchers

1. Prof. Ivan Bratko\*
2. Asst. Prof. Aleš Dobnikar\*
3. Prof. Bogdan Filipič
4. Prof. Matjaž Gams, Head
5. Dr. Anton Gradišek
6. Dr. Mitja Luštrek
7. Dr. Tomaž Šef

### Postdoctoral associates

8. Dr. Erik Dovgan\*
9. Dr. Hristijan Gjoreski, on leave 01.12.16
10. Dr. Matej Guid
11. Dr. Boštjan Kaluža
12. Dr. Miha Mlakar
13. Dr. Aleksander Pivk\*
14. Dr. Tea Tušar
15. Dr. Vedrana Vidulin, 11.11.16, transferred to Department E8

### Postgraduates

16. Jani Bizjak, B. Sc.
17. Robert Blatnik, M. Sc.
18. Božidara Cvetković, B. Sc.
19. Martin Gjoreski, B. Sc.
20. Vito Janko, B. Sc.
21. Tomaž Kompara\*, B. Sc.

22. Dr. Jana Krivec\*
23. Damjan Kužnar, B. Sc.
24. Martin Pečar, B. Sc., 01.12.16, transferred to Department E7
25. Dr. Rok Piltaver\*
26. Aleš Tavčar, B. Sc.
27. Jernej Zupančič, B. Sc.

### Technical officers

28. Martin Frešer, B. Sc., left 01.10.16
29. Gregor Grasselli, B. Sc.
30. Matej Krebelj, B. Sc., left 13.02.16
31. Jure Šorn, B. Sc.
32. Aljoša Vodopija, B. Sc.

### Technical and administrative staff

33. Grigory Evseev, B. Sc.
34. Vesna Koricki, B. Sc.
35. Mitja Lasič
36. Liljana Lasič
37. Blaž Mahnič, B. Sc.
38. Pavel Maslov, B. Sc.
39. Lana Zemljak

Note:

\* part-time JSI member

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11. Aljaž Kramberger, Rok Piltaver, Bojan Nemeč, Matjaž Gams, Aleš Ude, "Learning of assembly constraints by demonstration and active exploration", *Ind. rob.*, vol. 43, no. 5, pp. 524-534, 2016.
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14. Rob Patro et al. (14 authors), "A computational method for designing diverse linear epitopes including citrullinated peptides with desired binding affinities to intravenous immunoglobulin", *BMC bioinformatics*, vol. 17, pp. 155-13-155-13, 2016.
15. Rok Piltaver, Mitja Luštrek, Matjaž Gams, Sanda Martinčič-Ipšič, "What makes classification trees comprehensible?", *Expert syst. appl.*, vol. 62, pp. 333-346, 2016.

16. Aleš Tavčar, Csaba Antonya, Valentin Butila, "Recommender system for virtual assistant supported museum tours", *Informatika (Ljublj.)*, vol. 40, no. 3, pp. 279-284, 2016.
17. Niki Veček, Marjan Mernik, Bogdan Filipič, Matej Črepinšek, "Parameter tuning with Chess Rating System (CRS-Tuning) for meta-heuristic algorithms", *Inf. sci.*, vol. 372, pp. 446-469, Dec. 2016.
18. Jure Žabkar, Ivan Bratko, Janez Demšar, "Extracting qualitative relations from categorical data", *Artif. intell.*, vol. 239, pp. 54-69, Oct. 2016.

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1. Csaba Antonya, Silviu Butnariu, Matjaž Gams, "Haptic interface design for experiencing ancient works", In: *Delavnica e-Heritage: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 11.-12. oktober 2016, [Ljubljana, Slovenija]: zvezek F*, pp. 16-19.
2. Anne Auger, Dimo Brockhoff, Nikolaus Hansen, Dejan Tušar, Tea Tušar, Tobias Wagner, "Benchmarking MATLAB's gamultiobj (NSGA-II) on the bi-objective BBOB-2016 test suite", In: *GECCO comp'16: proceeding of the 2016 on Genetic and Evolutionary Computation Conference Companion, July 20-24, 2016, Denver, Colorado, USA*, pp. 1233-1239.
3. Anne Auger, Dimo Brockhoff, Nikolaus Hansen, Dejan Tušar, Tea Tušar, Tobias Wagner, "Benchmarking RM-MEDA on the bi-objective BBOB-2016 test suite", In: *GECCO comp'16: proceeding of the 2016 on Genetic and Evolutionary Computation Conference Companion, July 20-24, 2016, Denver, Colorado, USA*, pp. 1241-1247.
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7. Jan Bizjak, Hristijan Gjoreski, Matjaž Gams, "Deep learning for diagnosing heart problems from ECG signals", In: *BOOM 2016, 1st International Workshop on Biomedical Informatics with Optimization and Machine Learning in conjunction, BOOM 2016, with 25th International joint Conference on Artificial Intelligence (IJCAI), July 9, 2016, New York, USA*, 1 pp.
8. Jani Bizjak, Hristijan Gjoreski, Matjaž Gams, "Pametna ura za starejše", In: *Delavnica Elektronsko in mobilno zdravje: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10.-11. oktober 2016, [Ljubljana, Slovenija]: zvezek G*, pp. 10-13.
9. Jani Bizjak, Hristijan Gjoreski, Matjaž Gams, "Projekt IN LIFE v Sloveniji", In: *Delavnica Elektronsko in mobilno zdravje: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10.-11. oktober 2016, [Ljubljana, Slovenija]: zvezek G*, pp. 7-9.
10. Martin Bonchanoski, Hristijan Gjoreski, Jani Bizjak, Matjaž Gams, "Smartwatch fall detection", In: *Delavnica Elektronsko in mobilno zdravje: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 10.-11. oktober 2016, [Ljubljana, Slovenija]: zvezek G*, pp. 17-20.
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15. Erik Dovgan, "Multiobjective discovery of driving strategies using the SCANer Studio", In: *Slovenska konferenca o umetni inteligenci: zbornik 19. mednarodne multikonference Informacijska družba - IS 2016, 12. oktober 2016, [Ljubljana, Slovenija]: zvezek A*, pp. 21-24.
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

- Ivan Bratko, Dayana Hristova, Matej Guid, "Search versus knowledge in human problem solving: a case study in chess", In: *Model-based reasoning in science and technology: logical, epistemological, and cognitive issues*, (Studies in applied philosophy, epistemology and rational ethics, vol. 27), Lorenzo Magnani, ed., Claudia Casadio, ed., [S. l.], Springer, cop. 2016, pp. 569-583.

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- Azlan Iqbal, Matej Guid, Simon Colton, Jana Krivec, Shazril Azman, Boshra Haghighi, *The digital synaptic neural substrate: a new approach to computational creativity*, (Springer briefs in cognitive computation), [S. l.], Springer, cop. 2016.
- Boštjan Kaluža, *Machine learning in Java: design, build, and deploy your own machine learning applications*, Birmingham, Packt Publishing, 2016.

## PATENT APPLICATION

- Matjaž Gams, Hristijan Gjoreski, Mitja Luštrek, *Method and system for detecting a person driving a vehicle while using a mobile computing device*, GB2528877 (A), Intellectual Property Office, 02. 10. 2016.

## PATENT

- Matjaž Gams, Hristijan Gjoreski, Mitja Luštrek, *Method and system for detecting a person driving a vehicle while using a mobile computing device*, S124796 (A), Urad RS za intelektualno lastnino, 29. 02. 2016.

## MENTORING

- Rok Piltaver, *Constructing comprehensible and accurate classifiers using data mining algorithms*: doctoral dissertation, Ljubljana, 2016 (mentor Matjaž Gams; co-mentor Mitja Luštrek).
- Martin Gjoreski, *Continuous stress monitoring using a wrist device and a smartphone*: master's thesis, Ljubljana, 2016 (mentor Matjaž Gams; co-mentor Mitja Luštrek).
- Martin Frešer, *Analysis and prediction of ambiental data with machine-learning and recommender system for better air-quality in work-places*: master's thesis, Ljubljana, 2016 (mentor Dejan Lavbič; co-mentor Mitja Luštrek).
- Leon Noe Jovan, *Data preparation for municipal virtual assistant using machine learning*: master's thesis, Ljubljana, 2016 (mentor Matjaž Kukar; 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 undergraduate and doctoral studies programmes.*

## Modelling of basic thermal-hydrodynamic phenomena

Turbulent heat transfer was investigated by performing Direct Numerical Simulations, using the spectral element method and the computer code nek5000, within the European Commission (EC) project SESAME, dedicated to the thermal hydraulics of liquid metals. Simulations are being performed in the geometry of a backward-facing step, which will be implemented in one of the SESAME experiments. Inlet boundary conditions are obtained with prescribed mean mass flow rate and a "recycling method", while outlet boundary conditions are implemented with a method that prevents backflow into the domain.

Investigations of jet impingement cooling phenomenology were continued. Based on an analysis of an extensive Large Eddy Simulation (LES) database of a selected experimental case with multiple turbulent impinging jets, the instantaneous heat-transfer phenomenology was comprehensively interpreted and explained.

Conjugate heat-transfer simulations were started with the development of a wall-resolved LES model, using the open-source code Code\_Saturne and in collaboration with Electricité de France (EDF). The final goal is the development and qualification of LES models for detailed simulations of turbulent heat transfer in geometries where the penetration of turbulent fluctuations into solid walls must be predicted.

The flow in a fuel bundle with a grid spacer was simulated using the URANS (Unsteady Reynolds Averaged Navier-Stokes) turbulence model. The simulations have shown a clear decoupling of large vortices induced by the flow separation, which were explicitly simulated, and small scale turbulent vortices, which were modelled with a RANS turbulence model. The results were validated with the MATiS-H experiment (Measurement and analysis of turbulent mixing in sub-channels – horizontal) performed at the Korea Atomic Energy Research Institute.

Separated upward air-water flow in a vertical pipe, which is related to the flooding phenomenon during nuclear reactor accidents, was simulated using interface-capturing methods. The influence of the liquid inlet on the flooding wave frequency was investigated and a strong correlation between the two was demonstrated.

The basic phenomena of vapour explosion and debris bed coolability, which might occur during a hypothetical severe accident in a nuclear power plant if the hot reactor-core melt comes into contact with the coolant, were also investigated. Analyses of the material influence of the oxide and metallic corium on the ex-vessel vapour explosion in the cavity of a pressurized water reactor have shown that with metallic corium, stronger explosions may occur. We also continued with studies of vapour explosions in stratified melt-coolant configurations. The recently performed experiments in the PULiMS/SES facility (Royal Institute of Technology, Sweden) have revealed that strong stratified explosions may develop spontaneously. In order to investigate the premixed layer formation mechanisms in stratified conditions, a SES test with an underwater melt delivery has been proposed within the EC FP7 SAFEST project by an international user group led by JSI and EDF. The test resulted in a strong spontaneous explosion right after the initiation of the melt spreading. Analyses of X-ray images of the OECD SERENA KROTOS experiments (Commissariat à l'Énergie Atomique - CEA, France), in parallel with supporting MC3D code (Institut de Radioprotection et de Sûreté Nucléaire - IRSN, France) calculations, provided additional insights into the complex premixing processes. Apart from that, the potential of vapour explosions during melt-sodium interactions was also investigated.



Head:  
**Prof. Leon Cizelj**

**An experiment on hydrogen combustion, proposed by JSI and NRG, was performed in the HYMIT facility at Shanghai Jiao Tong University (China).**

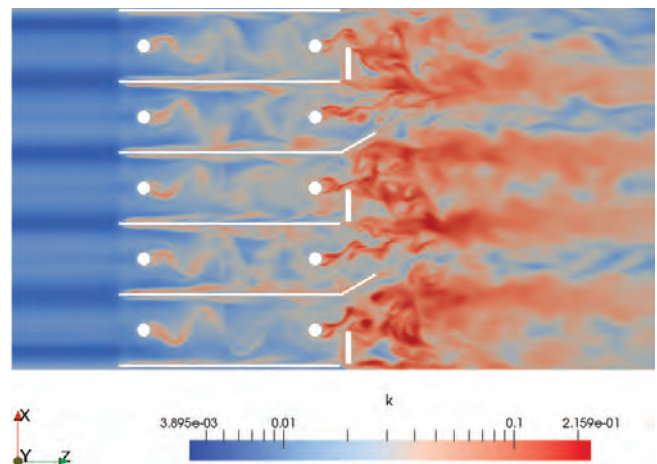


Figure 1: Enhancement of instantaneous turbulent kinetic energy for a mixing grid in the plane cut through a 5×5 rod bundle.

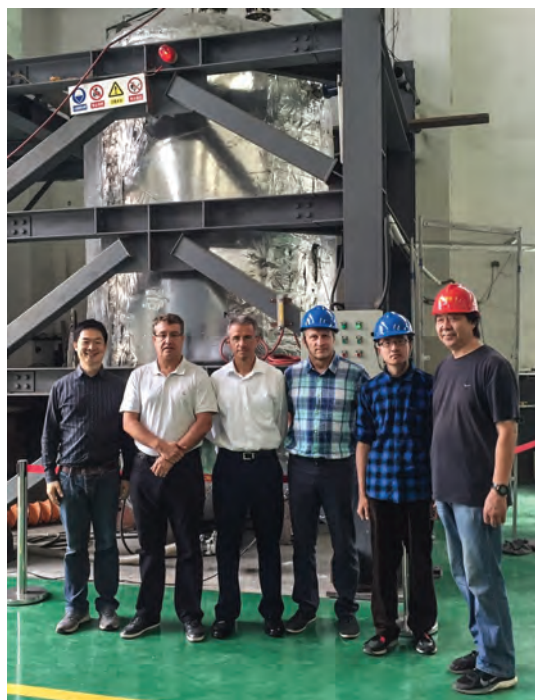


Figure 2: Execution of a hydrogen combustion experiment in the HYMIT experimental facility at Shanghai Jiao Tong University (China).

The analysis of experiments, dedicated to the film boiling regime, led to the proposal of an improved approach to model this boiling regime. The MC3D code was also used to perform simulations of recently performed PEARL experiments (IRSN), which are dedicated to debris bed coolability issues.

In the field of research on hydrogen combustion in NPP containment, an experiment on hydrogen deflagration was performed within the Chinese-EU project ALISA at Shanghai Jiao Tong University (China) in the HYMIT facility. The experiment specification was proposed by JSI and Nuclear Research and Consultancy Group (NRG, Netherlands). The results of the experiment are now being used for our further research on the theoretical modelling of hydrogen combustion. Apart from that, simulations of a similar experiment that we performed in 2012 at the Karlsruhe Institute of Technology (KIT, Germany) were continued with a modified combustion modelling, again in cooperation with NRG.

With regard to the new experimental laboratory for fluid mechanics and heat-transfer research under construction, there were important advances performed in an attempt to close the primary fluid loop. An important part of the test facility's instruments was installed and wired. However, most of the focus in the past year was dedicated to the design and construction of a unique test section that will allow for local heat-transfer coefficient measurements on a heated rod in an annulus during single-phase flow, flow boiling, convective condensation and critical heat flux, while allowing a visual inspection of the studied phenomenon at desired locations. The one-of-a-kind measuring device will allow for diabatic fluid flow measurements at controlled wall temperatures.

Within our current experimental activities, coolant temperature distributions in the cooling channels of the TRIGA research reactor were measured and compared with computational fluid dynamics (CFD) simulations. A simplified CFD model is being used for coupled neutronic and thermal hydraulic simulations of the experimental reactor.

#### Thermal-hydraulic safety analyses

The accident at the Fukushima Daichi nuclear power plant in 2011 demonstrated that external events may cause the loss of all active safety systems. Therefore, safety upgrade programs (SUP) for existing nuclear power plants were initiated. We demonstrated that a developed input model of a two-loop pressurized water reactor (PWR) for the TRACE thermal-hydraulic systems code can be used for an independent assessment of the RELAP5 computer code calculations, which were used in the frame of the Krško NPP SUP. As a demonstration, the response of a PWR to loss-of-coolant accident (LOCA) break spectrum of 12", 8", 6", 5" and 4" equivalent diameter cold leg breaks was simulated. Only passive components, i.e., accumulators, were assumed available, and the time available before significant core heatup was estimated.

The development of the thermal shielding concept for the demonstration fusion reactor DEMO was carried out within the frame of the EUROfusion project. A preliminary calculation of heat conduction loads from the thermal shield supports and from the magnet support was performed. The total power of the DEMO cryo-coolant system was predicted, taking into account thermal radiation and heat-conduction heat losses.

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### **We simulated loss-of-coolant and loss-of-cooling accidents in the spent-fuel pool of the Fukushima (Japan) nuclear power plant.**

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The overall efficiency of the cryo-cooling was optimised in terms of different cooling temperatures of the vacuum vessel and thermal shields.

In the frame of the NUGENIA+ Air SFP project, we participated in a benchmark simulation of loss-of-coolant and loss-of-cooling accidents in

the spent fuel pool of the Fukushima NPP. We developed a suitable model for the ASTEC system code, specifically for the ICARE module, which is used to simulate heat up and degradation of the reactor core.

Within the European CESAM project, we simulated five experiments of hydrogen combustion in a non-homogeneous atmosphere (both in terms of atmosphere composition as well as temperature) with upward and downward flame propagation, performed in the THAI experimental facility (Becker Technologies, Germany), with the ASTEC code. Although system codes use a volume-averaged description of the containment, they are suitable for the safety analyses of real plants.

#### Structural safety analyses

In cooperation with CEA, the recently developed micro-mechanical crystal plasticity model for neutron-irradiated stainless steel was re-calibrated by using a representative finite-element model of a realistic tensile specimen. The finite-element model was identified by extrapolating the results of tensile simulations on various finite aggregate models to a continuum limit. Using a representative model and a novel fitting approach, the adjustment of the model parameters was performed with respect to tensile measurements on 304L stainless steel up to the necking point.

Within the EC project SOTERIA and in collaboration with CEA, the normal stresses and cumulative plastic strains were calculated at grain boundaries in neutron-irradiated stainless steel for uniaxial tensile loading conditions. Polycrystalline simulations were performed on Voronoi and realistic steel-wire aggregates. Once rescaled by the macroscopic stress, the obtained intergranular stress distributions were found to be well approximated by a bi-modal master curve.

The uncertainties in the prediction of thermal fatigue lives of pipes subjected to turbulent fluid mixing were estimated using total-life and damage-tolerant approaches with an improved spectral loading method, developed at the JSI, for the generation of fluid-temperature histories. The influence of various fluid-flow parameters and heat-transfer coefficients on the predicted fatigue lives and crack growth were analysed.

We participated in two EC projects in the field of nuclear fusion. Within the WPDC project (diagnostic and control), the initial feasibility assessment was carried out on the divertor thermo-current measurement diagnostics for the DEMO fusion reactor. Maximum voltage differences were calculated along the divertor cassette for a given current power and various couplings of the divertor with vacuum vessel and divertor cooling pipes. A split-cassette design was shown to provide reasonably high voltage drops for plasma detachment control.

Within the PMI-PPPT-FU project (plant level system engineering), the initial concept design for the expansion joints between the vacuum vessel port and the cryostat in the DEMO reactor, referred as port duct bellows, was studied. The initial geometry of the bellows was defined and the first results on the mechanical stresses, due to gravity loading and relative movements of the connecting parts, were reported.

#### Probabilistic safety assessment

Within the EC ASAMPSA\_E project, which aims at promoting good practices for the identification of a combination of two correlated extreme external events having significant influences on nuclear safety with the help of probabilistic safety assessment (PSA), we studied how “extended PSA” can be developed efficiently, as well as specific problems, related to Level 2 PSA (expected frequency, quantity, composition, location, etc. of radioactive releases into the environment because of barrier failure and failure of containment systems). We also participated in the organisation of the ASAMPSA\_E end-user workshop. The purpose of the workshop was to review, together with end-users, comments and improvements provided during the review process of the preliminary ASAMPSA\_E reports. Regulatory bodies, nuclear power plant operators, technical organisations and research organisations, which work or are related to PSA, were involved in the review process.

#### Technical cooperation, consulting services and education

In 2016, the Department of Reactor Engineering cooperated in projects for industry as well. As an authorized institution for radiation and nuclear safety, we prepared a report with proposals for safety improvements to the Krško NPP, based on inspection activities on safety structures, systems and components during the plant 2016 outage. In addition, an independent evaluation of the modified Krško fuel design was performed. Mechanical changes to the fuel resulted in a change of critical heat flux and consequently influenced the results of the large-break loss-of-coolant-accident event analysis within the Updated Safety Analysis Report.

Members of the department are also actively involved in nuclear engineering undergraduate, 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 three years

1. B.Mikuž, I.Tiselj, Wall-resolved Large Eddy Simulation in grid-free 5 x 5 rod bundle of MATIS-H experiment, *Nuclear Engineering and Design*, 298 (2016), 64-77.
2. M.Tekavčič, B.Končar, I.Kljenak, Simulation of flooding waves in vertical churn flow, *Nuclear Engineering and Design*, 299 (2016), 214-224.
3. M.Leskovar, V.Centrih, M.Uršič, Simulation of steam explosion in stratified melt-coolant configuration, *Nuclear Engineering and Design*, 296 (2016), 19-29.

### Uncertainties in the prediction of the thermal fatigue lives of pipes, subjected to turbulent fluid mixing, were estimated using an improved spectral loading method developed at the JSI.

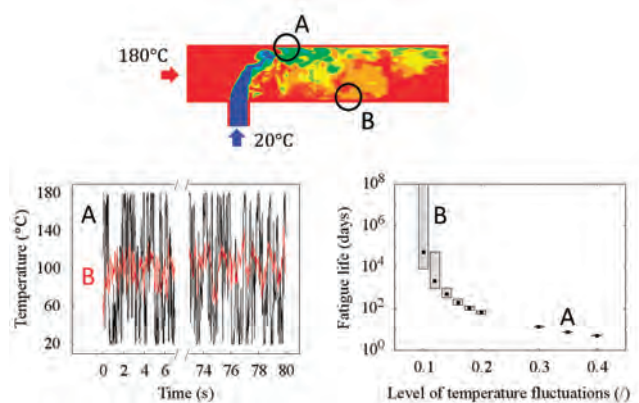


Figure 3: In a T-junction (top), synthetic fluid temperature signals (bottom left), generated with an improved spectral loading method developed at JSI, are used to predict fatigue lives as well as associated uncertainties (bottom right).



4. O.Costa Garrido, S.El Shawish, L.Cizelj, Uncertainties in the thermal fatigue assessment of pipes under turbulent fluid mixing using an improved spectral loading approach, *International Journal of Fatigue*, 82 (2016), 550-560.
5. M.Leskovar, M.Uršič, Analysis of PWR ex-vessel steam explosion for axial and side melt release, *Nuclear Engineering and Design*, 283 (2015), 40-50.
6. R.Henry, I.Tiselj, L.Snoj, Analysis of JSI TRIGA MARK II reactor physical parameters calculated with TRIPOLI and MCNP, *Applied Radiation and Isotopes*, 97 (2015), 140-148.
7. O.Costa Garrido, S.El Shawish, L.Cizelj, Stress assessment in piping under synthetic thermal loads emulating turbulent fluid mixing, *Nuclear Engineering and Design*, 283 (2015), 114-130.
8. A.Prošek, A.Volkanovski, Extended blackout mitigation strategy for PWR, *Nuclear Engineering and Design*, 295 (2015), 360-373.

### Awards and appointments

1. Oriol Costa Garrido: Winner prize for the best presentation of relevant research in nuclear fields (ENC 2016 conference, Warsaw, Poland), European Nuclear Education Network, Life-time predictions accuracy of the thermally fatigued pipes under turbulently mixing fluids
2. Oriol Costa Garrido: Best poster award (ICONE 24 conference, Charlotte, North Carolina, USA), American Society of Mechanical Engineers, Probabilistic prediction of fatigue life of pipes under turbulent fluid mixing
3. Tadej Holler: Best paper award (ICONE 24 conference, Charlotte, North Carolina, USA), American Society of Mechanical Engineers, Large-scale homogeneous hydrogen-air-steam deflagration experiment simulated using two turbulent flame speed closure models
4. Janez Kokalj, Matjaž Leskovar, Mitja Uršič: Best poster award (NENE 2016 conference, Portorož, Slovenia), Nuclear Society of Slovenia, Modelling of Debris Bed Coollability in Bottom Reflooding Conditions with MC3D
5. Matic Kunšek: Certificate; European master of nuclear engineering (IAEA General conference, Vienna, Austria), European Nuclear Education Network

### Organization of conferences, congresses and meetings

1. SOTERIA Project General Assembly, Jožef Stefan Institute Reactor Center, Ljubljana (29.-30.09.2016)

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## INTERNATIONAL PROJECTS

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| <ol style="list-style-type: none"> <li>1. Research of Conjugate Heat Transfer in Turbulent Pipe Flow<br/>Prof. Iztok Tiselj<br/>Electricite De France S.a.</li> <li>2. Overheating of Containers for Dry Storage of Spent Fuel after Full Blockage of Ventilation Channels<br/>Dr. Matjaž Leskovar<br/>Areva GmbH</li> <li>3. 7FP - CESAM; Code for European Severe Accident Management<br/>Asst. Prof. Ivo Kljenak<br/>European Commission</li> <li>4. 7FP - ASAMPESA_E; Advanced Safety Assessment: Extended PSA<br/>Dr. Andrej Prošek<br/>European Commission</li> <li>5. 7FP - ARCADIA; Assessment of Regional Capabilities for New Reactors Development through an Integrated Approach<br/>Prof. Leon Cizelj<br/>European Commission</li> <li>6. 7 FP - NUGENIAS-PLUS (AIR-SFP); Spent Fuel Pool Behaviour in Loss of Cooling of Loss of Coolant Accidents<br/>Asst. Prof. Marko Matkovič<br/>European Commission</li> <li>7. Better understanding and recognition of nuclear skills and qualifications<br/>Prof. Leon Cizelj<br/>University Politehnica of Bucharest</li> <li>8. Training and Tutoring for Experts of the National Regulatory Authorities and their Technical Support Organisations for Developing or Strengthening their Regulatory and Technical Capabilities - MC3.01/13<br/>Prof. Leon Cizelj<br/>Iter-consult Srl - Independent</li> <li>9. H2020 - SESAME; thermal hydraulics Simulations and Experiments for the Safety Assessment of Metal cooled reactors<br/>Prof. Iztok Tiselj<br/>European Commission</li> <li>10. H2020 - SOTERIA; Safe Long Term Operation of Light Water Reactors based on Improved Understanding of Radiation Effects in Nuclear Structural Materials</li> </ol> | <p>Prof. Leon Cizelj<br/>European Commission</p> <ol style="list-style-type: none"> <li>11. H2020 - ANNETTE; Advanced Networking for Nuclear Education and Training and Transfer of Expertise<br/>Prof. Leon Cizelj<br/>European Commission</li> <li>12. RU-FU, EUROFUSION; Research Unit - Administration and Services<br/>Dr. Boštjan Končar<br/>European Commission</li> <li>13. Education-ED-FU, EUROFUSION<br/>Dr. Boštjan Končar<br/>European Commission</li> <li>14. Diagnostic and Control-WPDC-PPPT-FU, EUROFUSION<br/>Dr. Samir El Shawish<br/>European Commission</li> <li>15. Plant Level System Engineering-PMI-PPPT-FU<br/>Dr. Boštjan Končar<br/>European Commission</li> <li>16. Investigation of Coolant Flow and Heat Transfer Characteristics in a High Temperature Gas-cooled Reactor<br/>Prof. Leon Cizelj<br/>Slovenian Research Agency</li> <li>17. MS-MZDR/16-1-B2-125; SNETP - Sustainable Nuclear Energy Technology Platform; SNETP General Assembly, Meeting of the Governing Board; Brussels, Belgium, 21.-23.3.2016, 19.-20.10.2016<br/>Prof. Leon Cizelj<br/>Slovenian Research Agency</li> <li>18. MS-MZDR/16-1-B2-053; General Assembly of the ENEN Association, President of the Governing Board; Paris, France, 13.-14.10.2016, 15.-16.12.2016<br/>Prof. Leon Cizelj<br/>Slovenian Research Agency</li> <li>19. MS-MZDR/16-1-B2-112; General Assembly of the ETSO Association, Member of the Governing Board; Paris, France, 13.-14.7.2016; Munchen, Germany, 7.-9.11.2016<br/>Prof. Leon Cizelj<br/>Slovenian Research Agency</li> <li>20. Investigation of stratified steam explosions<br/>Dr. Matjaž Leskovar<br/>Slovenian Research Agency</li> </ol> |
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21. Towards quantitative prediction of stress corrosion cracking initiation stress threshold for PWR's internals  
Dr. Samir El Shawish  
Slovenian Research Agency

Prof. Leon Cizelj  
ANDRA - The French National Radioactive Waste

## RESEARCH PROGRAM

1. Reactor engineering  
Prof. Leon Cizelj

## R&D GRANTS AND CONTRACTS

1. Feasibility of the Modelling of Interaction between Molten Corium and Sodium in the MC3D Software for SFR Applications  
Dr. Mitja Uršič  
Institut De Radioprotection Et De
2. JOPRAD: Joint Programming on Radioactive Waste

## NEW CONTRACTS

1. Cooperation in an international CAMP program  
Dr. Andrej Prošek  
Nuklearna Elektrarna Krško
2. Independent Evaluation of Modified Krško 16x16 VANTAGE+Fuel design fully in accordance with NEK Technical Specification SP-ES1250 Rev.0  
Dr. Matjaž Leskovar  
Nuklearna Elektrarna Krško d. o. o.
3. Understanding and managing the processes related to SFP under loss of cooling and loss of coolant accident scenario  
Assist. Prof. Marko Matkovič  
Nuklearna Elektrarna Krško
4. Joint Expert Assessment of the Outage Activities, Interventions and Tests during a shutdown and refueling outage 2016  
Dr. Mitja Uršič  
Elektroinštitut Milan Vidmar

## VISITORS FROM ABROAD

1. Ms. Zoya Trafimchik, Ms. Ylyana Kruk, Dr. Natalia Lukashenko: Department of Nuclear Radiation Safety of the Ministry of Emergency Situations of the Republic of Belarus (Minsk, Belarus), 09.09.2016
2. Mr. Virgil Aurelian Iliescu: National Commission for Nuclear Activities Control - CNCAN (Bucharest, Romania), 09.09.2016
3. Dr. Asif Arastu, Mr. Clayton Smith, Mr. Robert Stakenborghs: The American Society of Mechanical Engineers - ASME (USA), 09.09.2016
4. Dr. Sofiane Benhamadouche, Dr. Martin Ferrand: Electricité de France (EDF) Research and Development (Chatou, France), 24.-26.10.2016
5. Mr. Stefan Reisinger, Mr. Matjaž Kavčič: Embassy of the United States of America in Slovenia (Ljubljana, Slovenia), 15.12.2016

## STAFF

### Researchers

1. Prof. Leon Cizelj, Head
2. Dr. Samir El Shawish
3. *Ljubo Fabjan, M. Sc., retired 01.09.16*
4. Asst. Prof. Ivo Kljenak
5. Dr. Boštjan Končar
6. Dr. Matjaž Leskovar
7. Asst. Prof. Marko Matkovič
8. Dr. Andrej Prošek
9. Prof. Iztok Tiselj
10. Dr. Mitja Uršič
11. *Dr. Andrija Volkanovski, on leave 16.05.15*

### Postdoctoral associates

12. Dr. Oriol Costa Garrido
13. Dr. Martin Draksler
14. Dr. Cedric Cyril Henri Flageul
15. Dr. Blaž Mikuž

### Postgraduates

16. *Ovidiu-Adrian Berar, B. Sc., left 01.05.16*
  17. Romain Claude Francis Henry, B. Sc.
  18. Tadej Holler, B. Sc.
  19. Janez Kokalj, B. Sc.
  20. Rok Krpan, B. Sc.
  21. Matic Kunšek, B. Sc.
  22. Jure Oder, B. Sc.
  23. Matej Tekavčič, B. Sc.
- ### Technical officers
24. Sandi Cimerman, B. Sc.
  25. Andrej Sušnik, B. Sc.
- ### Technical and administrative staff
26. Tanja Klopčič
  27. *Urška Knjific Terze, B. Sc., left 01.04.16*
  28. Zoran Petrič, B. Sc.
  29. Nina Rehar, B. Sc.

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sensitivity study of a developed model", *Reliab. eng. syst. saf.*, vol. 148, pp. 11-20, 2016.

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1. Vasilij Centrih, Matjaž Leskovar, "Analysis of x-ray images in SERENA KROTOS experiments with premixing simulations", In: *Proceedings, 25th International Conference Nuclear Energy for New Europe - NENE 2016*, Portorož, Slovenia, September 5-8, 2016, pp. 811-1-811-9.
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## SCIENTIFIC MONOGRAPH

1. Andrija Volkanovski, Antonio Ballesteros Avila, Miguel Peinador, *European clearinghouse on operating experience feedback for nuclear*

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## PROFESSIONAL MONOGRAPH

1. Andrej Prošek, Andrija Volkanovski, *RELAP5 analysis of mitigation strategy for extended blackout power condition in PWR RELAP5 analysis of mitigation strategy for extended blackout power condition in PWR: prepared as part of The Agreement on Research Participation and Technical Exchange Under the Thermal-Hydraulic Code Applications and Maintenance Program (CAMP)*, (International agreement report, NUREG/IA-0467), Washington, U.S. Nuclear Regulatory Commission, 2016.

## MENTORING

1. Oriol Costa Garrido, *Random thermal loads in the thermal fatigue assessment of nuclear piping*: doctoral dissertation, Ljubljana, 2016 (mentor Leon Cizelj; co-mentor Iztok Tiselj).
2. Blaž Mikuž, *Modelling of turbulent flow in a fuel assembly of pressurized water reactor*: doctoral dissertation, Ljubljana, 2016 (mentor Iztok Tiselj).
3. Tomaž Skobe, *Analysis of steam explosion in flooded reactor cavity*: master's thesis, Ljubljana, 2016 (mentor Matjaž Leskovar).
4. Luka Klobučar, *Simulation of thermal loading on divertor cassette in fusion reactor*: master's thesis, Ljubljana, 2016 (mentor Iztok Tiselj; co-mentor Boštjan Končar).
5. Janez Kokalj, *Modelling of debris bed reflooding in PEARL experimental facility*: master's thesis, Ljubljana, 2016 (mentor Iztok Tiselj; co-mentor Mitja Uršič).
6. Rok Krpan, *Simulation of a low-momentum steam jet interaction with a light gas layer in a containment facility*: master's thesis, Ljubljana, 2016 (mentor Ivo Kljenak).



# REACTOR INFRASTRUCTURE CENTRE

# RIC

***The Reactor Infrastructure Centre (RIC) incorporates a TRIGA Mark II research reactor and a Hot Cells Facility. The reactor, operating since 1966, is used for neutron research, training and for radioactive isotope production. 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 regular radiological measurements of radioactive waste and irradiated samples.***

***Besides operating and maintaining the reactor, the members of the reactor staff participate in other activities requiring specialists skilled in work with sources of radiation and in reactor technology, such as the servicing of industrial radioactive sources and surveillance of the fuel management in NPP Krško.***



Head:  
**Prof. Borut Smodiš**

The reactor operated in accordance with a programme approved by the Heads of the RIC and the Radiation Protection Unit – RPU (SVPIS in Slovene) for each week. In 2016 the reactor operated 134 days and produced 104.8 MWh of heat. Altogether, six pulses were carried out. A total of 758 samples were irradiated in the rotary specimen rack and 35 in the pneumatic transfer system.

The reactor operators supported 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 2016 the reactor was mainly used as a neutron source for neutron-activation analysis, 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 Department of Experimental Particle Physics – F9. The Reactor Physics Department – F8 used the reactor for experiments in reactor physics, and Reactor Engineering Department – R4 used the reactor for thermal-hydraulic experiments.

The shutdown reactor, being a powerful source of gamma radiation, was repeatedly used for testing the resistance of electronic components to radiation.

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 activities:

- Reactor physics and neutronics;
- Activation analysis;
- Research on the radiation damage of semiconductors;
- Neutron dosimetry and spectrometry;
- Activation of materials, nuclear waste and decommissioning;
- Radiation hardness studies;
- 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.

A series of experiments involving the irradiation of various detectors were conducted in the framework of a collaboration between F8 and the French Alternative Energies and Atomic Energy Commission (CEA), Cadarache.

In the scope of the NATO SPS project E-SiCure (<http://e-secure.web.ua.pt/>) aimed at engineering silicon carbide material for detectors of special nuclear material for border and port security, in which F8 is involved, the reactor was used to perform test irradiations of silicon carbide samples to study the neutron-induced defects in the material.

Within the F4E project “Gas Production Experiment and TBM Nuclear Instrumentation” the reactor was used to perform irradiations of TLDs and Al-Mn activation foils to determine the possibility of tritium production monitoring using the  $^{55}\text{Mn}(n,\gamma)$  nuclear reaction.

In collaboration with R4 temperature measurements in the cooling channels of the reactor core were carried out.

In collaboration with F8 and F9, the reactor channel no. 6 was rearranged so as to allow for irradiating larger samples with neutrons.

Preparations for the Krško Nuclear Power Plant (NPP) reactor pre start-up tests were also conducted at the TRIGA reactor.

Since 2011, The TRIGA reactor participates in the FP7 AIDA (Advanced Infrastructures for Detectors and Accelerators) project that brings together advanced European infrastructures for future particle-physics experiments. In the framework of the international project “*Horizon 2020 - the AIDA-2020 GA No. 654168, Task 15.5 - Irradiation Facilities*” a contract was signed, together with F8, for the period from 1 May 2015 until 31 October 2016.

In the field of training, different lectures and practical exercises were conducted at the reactor. The participants were students from the following Slovenian universities: Faculty of Mathematics and Physics, Faculty of Electrical Engineering (University of Ljubljana) and Faculty of Energy Technology (University of Maribor). To carry out the exercises, the reactor was used for about three months, the average number of participants per experiment was 10. All the exercises were performed by our personnel in collaboration with F8.

The reactor will also be 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 14 November 2016 to 11 April 2017, and attended by four participants.

In December, a course on the “Requirements and Safety Evaluation of Research Reactors” within the project Instrument for Nuclear Safety Cooperation (INSC) was organized together with the Nuclear Training Centre. The course was held from 5 to 9 December; it was attended by 12 trainees.

In 2016 the reactor celebrated the 50<sup>th</sup> anniversary of its safe operation. A ceremony was held on 31 May 2016, attended by about 120 invitees from various fields related to the nuclear field.

In the last week in May the reactor staff hosted a TV crew from the *Radio-Television Slovenia* that was following up on the reactor-related activities by filming a documentary about the reactor. The film was broadcasted on the Slovenian national television in November.

In 2016, there were more than 40 group visits to the reactor. The visitors were mainly foreign scientists, students and 33 groups of schoolchildren. Their total number was more than 1600. In March the *Jožef Stefan Institute's Open Days* were organized, during which the reactor was visited by around 200 people.

## Organization of conferences, congresses and meetings

1. Research reactor operating group meeting, 26th Annual Meeting, Ljubljana, 18–21 May 2016.



*A ceremony for the 50th anniversary of the safe operation of the TRIGA Mark II research reactor*

## INTERNATIONAL PROJECTS

1. H2020 - AIDA-2020; Advanced European Infrastructures for Detectors at Accelerators  
Prof. Borut Smodiš  
European Commission

Anže Jazbec, B. Sc.  
National Nuclear Research Center

## R & D GRANTS AND CONTRACTS

1. Irradiation for FT-TIMS Method at the JSI TRIGA Mark II Reactor  
Asst. Prof. Luka Snoj
2. Irradiation and Analysis of Nano SiC Samples

## NEW CONTRACT

3. Processing and preparation of radioactive waste for the purpose of storage  
Prof. Borut Smodiš  
ARAO

## VISITORS FROM ABROAD

1. Ms. Zoya Trafimchik, Ms. Ylyana Kruk and Dr Natalia Lukashenka, Department of Nuclear Radiation Safety of the Ministry of Emergency Situations of the Republic of Belarus – Gosatomnadzor, Minsk, Republic of Belarus; and Mr. Virgil Aurelian Iliescu,

National Commission for Nuclear Activities Control – CNCAN, Bucharest, Romania, 9 September 2016 (Belarus Scientific visit at Jožef Stefan Institute under IAEA technical cooperation programme).

## STAFF

### Researcher

1. Prof. Borut Smodiš, Head

### Postgraduates

2. Anže Jazbec, B. Sc.

### Technical officers

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.
8. Nina Udir, B. Sc.

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2. Petra Planinšek, Borut Smodiš, Ljudmila Benedik, "Simultaneous determination and uptake assessment of selected radionuclides in plants grown in substrate contaminated with U-mill tailings", *J. radioanal. nucl. chem.*, vol. 309, no. 1, pp. 351-365, 2016.
3. Sebastjan Rupnik, Borut Smodiš, "Automation of a TRIGA-type pneumatic transfer system", *J. radioanal. nucl. chem.*, vol. 309, iss. 1, pp. 107-113, 2016.

### PUBLISHED CONFERENCE CONTRIBUTION

1. Sebastjan Rupnik, "Posodobitev standardne pnevmatske pošte na reaktorju TRIGA", In: *Zbornik 3. konference mladih z Odseka za reaktorsko fiziko (F8) Instituta Jožef Stefan: povzetki prispevkov, predstavljenih na konferenci v Reaktorskem centru Podgorica, 29. februarja 2016*, pp. 23-25.
2. Luka Snoj, Igor Lengar, Anže Jazbec, Vladimir Radulović, Gašper Žerovnik, Aljaž Kolšek, Patrick Sauvan, Francisco Ogando, Javier Sanz, Andrej Trkov, "Feasibility study of installing a thermal to 14 MeV

neutron converter into a research nuclear reactor", In: *Conference proceedings*, Berlin, 2016, 12 pp.

3. Marko Štrok, Borut Smodiš, Darja Mazej, "<sup>210</sup>Pb - from interference to advantage in <sup>210</sup>Pb determination with liquid scintillation counter", In: *Proceedings of the 20th International Conference on Radionuclide Metrology and its Applications, 8-11 June 2015, Vienna, Austria*, (Applied radiation and isotopes, vol. 109, 2016), pp. 296-300.

### INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Jernej Jerman, Andrej Lešnjak, Luka Snoj, Borut Smodiš, "Inspection of the TRIGA reactor tank", In: *History, development and future of TRIGA research reactors*, (Technical report series, no. 482), Vienna, IAEA = International Atomic Energy Agency, 2016, 10 pp.
2. Borut Smodiš, Luka Snoj, "The JSI TRIGA Mark II reactor, Slovenia", In: *History, development and future of TRIGA research reactors*, (Technical report series, no. 482), Vienna, IAEA = International Atomic Energy Agency, 2016, pp. 76-89.

### MENTORING

1. Petra Planinšek, *Plant uptake of selected natural radionuclides from contaminated environment: doctoral dissertation*, Ljubljana, 2016 (mentor Borut Smodiš; co-mentor Ljudmila Benedik)..





# NETWORKING INFRASTRUCTURE CENTRE

# NIC

***The Networking Infrastructure Centre (NIC) is responsible for the administration, development, management and expansion of the core network, ICT services and infrastructure for the Jožef Stefan Institute. It also supports the development of the computational, communication, data and security infrastructure for our research departments, centres and services.***

The NIC's main mission is to maintain the computing networks, services and hardware necessary to support the operation of research departments, programmes, groups and projects at the Jožef Stefan Institute. We provide a high level of connectivity to and integration with local and international communication networks and infrastructures, but we also deliver ICT support for research activities at the Jožef Stefan Institute, including the development, management and administration of the ICT infrastructure, computing 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 is responsible for the development, management, administration and support of the physical networking infrastructure for the Institute. It delivers support for local networks so as to ensure local and internet connectivity for users and services at the Institute. This task includes the management of wireless networks at the Institute locations and also 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 2016 we continued our on-going extension and optimisation of the physical network, cabling installations, active equipment and wireless access points installations and equipment upgrades (specifically core backbone network routers). We expanded the network and its support for virtual network links used for a number of internal networks, (super) computing clusters and virtual machine farms. We continued our work on expanded IPv6 protocol stack feature support and optimizations to the Institute backbone network.

The load on our additional 10 Gbit/s connection to 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) has steadily increased, prompting us to upgrade the capacity of the connection to  $2 \times 10$  Gbit/s between the Institute and ARNES, and  $3 \times 10$  Gbit/s between ARNES and LHCONE over the GÉANT network.

In the scope of the IR Optika at Arnes, we have been able to provide optical connectivity to the Hard Coatings Center in Domžale and to completely integrate their network with the Institute's network.

**Monitoring:** New components and services have been continuously integrated with existing traffic, event and status-monitoring infrastructure, implemented on the basis of software packages Nagios, Ganglia, Cacti, Observium and a customised dynamic analytical visualisation package built with Kibana and Elasticsearch as a backend. In combination with internally developed solutions and our internally developed system for environmental monitoring the monitoring system enables us to react to usage fluctuations and unexpected events in the domain of web services, security policies, firewalls, authentication and authorization, network time systems e-mail delivery, analysis, processing and security systems, physical machine sensory status, environmental data, power line data, etc.

**Wireless network:** We strive to improve the coverage and density of our wireless networks by adding a number of smaller wireless access points. This allows us to alleviate the effect of increasing numbers of users and devices and their more frequent and more critical usage patterns.

**IPv6 support:** Support for the IPv6 protocol stack across all the network segments is crucial in our long-term strategy for alleviating the load on the already mostly spent IPv4 address pool. Continuous upgrading and improvements in the network router protocol stack provides flexible support for new protocols, where IPv6 support and expanded use is our core strategy.



Head:  
**Vladimir Alkalaj, M. Sc. \***

**A modern up-to-date 10 Gbit/s network backbone, the IPv6 protocol and dedicated external links are 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.**

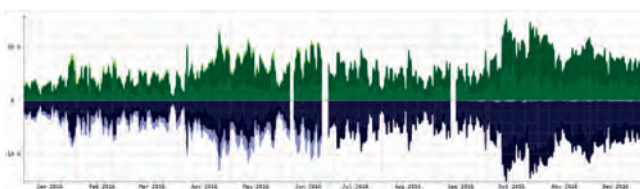


Figure 1: Gradually increasing network traffic over the LHCONE link during 2016 (from Observium monitoring).

\*Photo by Sašo Radelj

**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 implemented with dynamic management and configuration of active deep packet inspection firewall systems and routing configurations, with the exception of dedicated links where passive measures (configuration, filtering and supervision) are used. Constant dynamic supervision, traffic monitoring and event analysis is needed to ensure suitable security in the complex constraints and requirements of an open

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**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.**

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academic network that collide with current security considerations due to the increased detection of threats from the outside network. Therefore, ensuring the secure and open environment requires disproportionate increases in equipment capabilities and efforts in the dynamic security policy configuration, event monitoring and analytics.

Since the NIC is responsible for the security of the ICT infrastructure of the institute, we are active members of relevant institutions and groups, notably the national security response centre SICERT, FIRST (Forum of Incident Response and Security Teams) and EGI CSIRT (European Grid Initiative distributed computing security incident response team). We also take part in 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 the EU Grid PMA (EU Grid Policy Management Authority) and IGTF (Interoperable Global Trust Federation). We participate in the work of Slovenian network technology and security association SINOG (Slovenian Network Operators Group) and supported the organization by hosting two of the technical workshops at the Institute this year.

*E-Mail:* In the area of e-mail security and protection against undesired or malignant messages we have continued with our in-house software development, notably of the SpamAssassin package, and with continuous improvements in the support for international character sets in domain-name handling and e-mail message protocol stacks.

*Cryptography and certification:* We have continued with the gradual integration of DNSSEC-signed internet domain names using automated mechanisms for the verification of the signatures and with 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 DigiCert server certificates, courtesy of Arnes support, have been issued for services that are offered to the general public, since DigiCert certificates are recognised by the major operating systems and browsers. The number of users of our VPN infrastructure has been steadily increasing, in particular

also for connections to the user network at the Reactor Infrastructure Centre Podgorica. The system is not used only by researchers at foreign conferences and exchanges who have to deal with foreign networks that block certain types of connections, but is also more frequently used by users who are working from their homes and users that need it for access to on-line resources, such as scientific publication repositories. To alleviate the need of VPN for this common use case, we have worked with the Science Information Centre in an on-going effort to ensure accessibility of scientific publications using the eduGAIN single-sign-on federation credentials.



Figure 2: New server racks in the Jožef Stefan Institute Computing Centre at Teslova

**ICT services.** The NIC provisions, develops and maintains a number of core and some secondary 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 (main Institute web server, web hosting for users, departments and projects, a web directory). Secondary ICT services are provided for the support of certain core or specific activities at the Institute, 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, Google Play and Microsoft Store). The software development repository has stood out by attracting a large number of new users in the last year. 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 2015 we have established a new dedicated computing centre in the Technology Park building at Teslova. We have moved the majority of computationally-intensive infrastructure from our data centre at NIC during 2015 and 2016 this new data centre along with the installation of the new common supercomputing cluster, to better use the modern cooling, electrical and security systems and ample room for future growth. The NIC computing centre, on the other hand, has since been able to provide cooling, network facilities and high-performance uninterrupted power supply not only for critical services, but also for less computationally-intensive servers from several departments. We have also expanded our web-hosting activity (over 75 distinct virtual servers) and started deploying a test bed for virtualised hosting. The increased load on our personnel due to 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 is gaining popularity since it gives our users easier access to 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, network supercomputing, grids and HPC 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 founding 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 supercomputing grid network services and coordinates work with international infrastructure projects and collaborations.

In 2016, New System Cluster (NSC), the common computing cluster in the new facilities of the Jožef Stefan Institute's Computing Centre Teslova, has seen a very noticeable increase in usage and the number of users. The new cluster with 1984 64-bit computing cores, 16 GPGPU accelerators (NVIDIA Kepler 40), almost 9 TB RAM and 90 TB disk storage is far from the biggest cluster at the Institute, but it is an important step in the evolving traditions of supercomputing at the Jožef Stefan Institute, since it is available to all the researchers at the Institute and is thus providing an important modern computing platform to all of our departments. As a common infrastructure, it is instrumental in forwarding collaboration among departments with their own computing facilities and among researchers and groups with similar software requirements or computational problems that can be solved in an environment that can support supercomputing and high-throughput computing. In the context of this work, we have continued with support for users of JSI clusters and with work on 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.

In the domain of network computing we have been most involved with Slovenian National Grid Initiative (SLING), but we also worked with in the European Grid Initiative EGI (with 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 different services of Slovenian national node, ELIXIR – collaboration with the national node and the European collaboration). SLING has supported a number of research projects and applications in 2016, 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 administration of required run-time environments.

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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. A new common facility is an important step further for collaboration in the field of high-performance and network computing at JSI fostering interdepartmental collaboration.**

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*Figure 3: Water-temperature gauges on the cooling-system pipes in the Jožef Stefan Institute Computing Centre at Teslova*

## STAFF

### Technical officers

1. Vladimir Alkalaj, M. Sc., Head
2. Dr. Jan Jona Javoršek
3. Barbara Krašovec, M. Sc.
4. Mark Martinec, B. Sc.

### Technical and administrative staff

5. Ivan Ivanjko
6. Janez Jezeršek
7. Matjaž Levstek
8. Janez Srakar
9. Matej Wedam

## BIBLIOGRAPHY

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### PROFESSIONAL MONOGRAPH

1. Borut Bohanec, Mišo Alkalaj, *Kaj je res o GSO*, 2. dopolnjena izd., Ljubljana, Orbis, 2016.
2. Borut Bohanec, Mišo Alkalaj, *Yes to GMOs!: for us and the environment*, Ljubljana, Geanetic, 2016.

# SCIENCE INFORMATION CENTRE

# SIC

*The Jožef Stefan Institute Science Information Centre is the central Slovenian physics research library and the largest research library in Slovenia. Our main tasks are the acquisition, archiving, and loan of books and periodicals, and the input, update and control of bibliographic data of the Institute'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 4000 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**

## STAFF

### Technical officers

1. Dr. Luka Šušteršič, Head
2. Marjan Verč, M. Sc.

### Technical and administrative staff

3. Suzi Korošec, B. Sc.
4. Jasna Malalan
5. Katarina Modic, B. Sc.

6. Alenka Ana Stante, B. Sc.
7. Jože Škulj
8. Branka Štrancar
9. Ana Tratnik
10. Nada Tratnik
11. Saša Žnidar, B. Sc.



# ENERGY EFFICIENCY CENTRE

# EEC

*The basic activities of the Energy Efficiency Centre are in efficient energy use, long-term planning in energy and the reduction of greenhouse-gases emissions. The centre is a focal point for the collection and transfer of energy-efficiency technologies to energy users, the state, energy service and equipment providers, and other interested agencies. At the same time, it covers the environmental effects of energy use and conversion. The most significant part of the EEC's activities is thus cooperation with state institutions in the preparation of strategic documents and legislation in the field of efficient energy use, energy planning, distributed electricity production, and emissions trading. Nevertheless, it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as also being more and more involved in European research projects.*



Head:  
**Stane Merše, M. Sc.**

## Energy and the environment

In 2016 the Energy Efficiency Centre with its professional work ensured high-quality support to ministries in the preparation of the strategic development documents and transfer of EU legislation in the field of energy planning, energy efficiency, use of renewables and greenhouse-gases emissions and the reduction of other pollutants.

Slovenia has ambitious goals in the framework of climate energy policy regarding an increase of energy efficiency, the exploitation of renewable energy sources (RES) and a reduction of greenhouse-gases emissions. Energy efficiency is a priority field to achieve these goals, in accordance with the demands of the European Commission and the directive on energy efficiency (2012/27/EU). In accordance with this directive a report on carrying out the Action plan for energy efficiency for the period 2014–2020 was elaborated. The EEC also cooperated in the updating of the Action plan for renewable sources for the period 2010–2020 and inclusion in the procedure for the integrated assessment of impacts on the environment. The EEC was also included in the updating of the national long-term strategy for the promotion of investments in the energy renovation of buildings.

The EEC cooperates with the Statistical Office of the Republic of Slovenia, where it prepares a model calculation for fuels and energy use in households for the national energy statistics.

Also in 2016, the centre continued with activities of the state referential centre for energy with the preparation of an expanded set of indicators for energy and the environment.

In the field of greenhouse-gases emissions reduction, the activities of the Centre for the Ministry of Environment and Space focused on the preparation of the Second annual report on carrying out the Operative programme of measures for the reduction of GHG emissions for the period 2013–2020, updating of GHG emissions projections by 2035 and the preparation of analytical bases for international reporting in the framework of the MMR mechanism. A professional support for the design of goals and national policy concerning pollutants from the NEC directive up to 2030 continued and a detailed study of transit road and impacts on motor fuel sales in Slovenia was elaborated (Figure 1).

## Promotion of efficient energy use and energy consulting

The Energy Efficiency Centre in 2016 continued with its training activities where the ninth cycle of energy managers training was successfully concluded within the European programme EUREM. Due to a very positive reaction of participants and their interest (in Slovenia there is already more than 190 energy managers with 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 in competitiveness and development restructuring.**

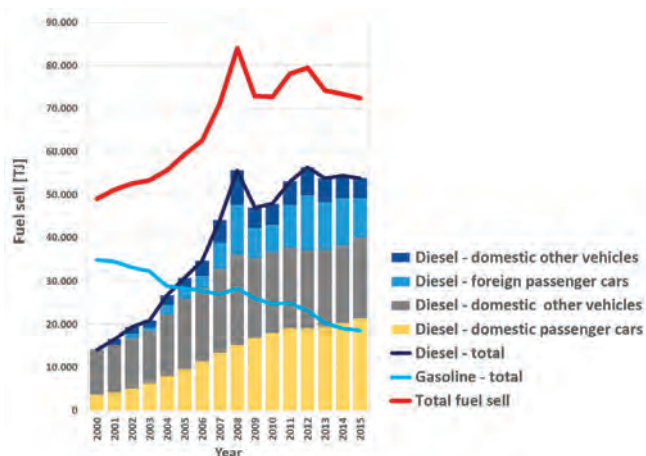


Figure 1: Trends of fuel sales in road transport in Slovenia - increase of diesel fuel use for personal sales vehicles and transit transport.





Figure 2: Four European award EUREM winners in 2016: Goran Matešić (Luka Koper), Drago Zupanc (Maksim), Kristijan Plesnik (Metal Ravne) and Jani Uranič (Xella porobeton) and their mentors at the Annual conference of European energy managers in Berlin

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.

This year an intensive development of the GIS tool for the spacial analysis of heat consumption in buildings (“heatmap”) has been going on. With the elaboration of spacial analysis of heat use and production concept for the preparation of the local energy concept it has been tested as a pilot project in the Municipality of Maribor (Figure 3).

In 2016 the Energy Efficiency Centre carried out several consulting tasks in industry and the public sector, where with the study of optimization of energy system started the cooperation with the company KOTO. The professional cooperation with Luka Koper, Energetika Ljubljana, BTC, etc. continued. For the company Petrol Energetika Ravne an elaboration of a study for the introduction of advanced energy services for industry and the local community, which are based on smart energy networks, started.

The centre continued professional cooperation with the company Petrol d.d. in carrying out the largest programme of large consumers to ensure energy savings for end users. The centre prepared the programme for the eighteenth conference “Energy Managers Days”, the annual meeting of energy managers with more than 200 participants confirms the quality and public profile of the EEC professional work.

### International cooperation

In 2016 the EEC carried out as many as 7 international projects, financed from the European Union resources in the framework of HORIZON 2020 and programme Intelligent Energy for Europe.

Projects cover activities in the fields of:

- compiling and elaboration of current data on renewable energy sources use (EurObserv`ER Barometer),
- carrying out the EU directive on energy efficiency (CA - EED),
- carrying out the EU directive on renewable energy sources (CA - RES),
- monitoring of indicators for energy use and energy efficiency in the EU (ODYSSEE MURE 2012).
- Energy contracting Plus (EPC Plus)
- Promotion of the introduction of energy contracting in the public and private sectors in the EU (guarantEE),
- Tool for the evaluation of the suitability of integrated energy retrofit (ENERFUND).

Projects include cooperations with research and development organisations from Europe with a strong emphasis on concrete applications and the promotion of energy efficiency. In the framework of each project the EEC staff took part in numerous foreign professional meetings and visits.

## Some outstanding achievements in 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, Letrika–Mahle, BTC, KOTO, etc.).
3. In the framework of the European project Transparens the EEC led, very successfully, the preparation of the European code of Conduct for energy contracting. The Code identifies the basic values and principles, which are of key importance for the successful preparation and carrying out of projects with third-party financing. The Code was very successfully accepted at the European level and currently already has 171 signatories, among them also the European association of companies for energy services (eu.ESCO) and the European federation for intelligent services of energy efficiency (EFIEES), supported also by the European Commission. In Slovenia the code was already tested in practice in a project of integrated energy renovation of the municipal building of the municipality Brda.



Figure 3: Spacial analysis of heat use in the area of Maribor: annual heat use in buildings, space density of heat use, types of heating appliances and energy infrastructure (distribution network of district heating and natural gas).

## Awards and appointments

1. Award TARAS – for successfully carrying out the project for the useful exploitation of waste heat in the steel industry in a district heat system in Ravne na Koroškem, which is a recognition for the most successful cooperation of economic and scientific research work

## Organization of conferences, congresses and meetings

1. Energy Managers Days 2016 – 18th meeting of Slovenian energy managers, Portorož, 19. – 20. 4. 2016
2. Partnerships of small and medium enterprises (SMEs) for standardized energy contracting, Ljubljana, 14.10.2016
3. European energy managers, Ljubljana, 13.-15.1.16, 2.-4.3.16, 16.-18.3.16, 12.-15.4.16



Figure 4: EEC and companies Petrol Energetika and Metal Ravne were awarded a prize TARAS for successfully carrying out a project for the useful exploitation of waste heat from the steel industry in the system of district heating in Ravne na Koroškem, which is a recognition for the most successful cooperation of economy and scientific research work in the field of innovations, development and technologies.

## INTERNATIONAL PROJECTS

1. IEE; EurObservER, The EurObserv'ER Barometer (2013-2016)  
Matjaž Česen, B. Sc.  
European Commission
2. H2020 - EPC\_PLUS; Energy Performance Contracting Plus  
Damir Staničič, M. Sc.  
European Commission
3. H2020 - ENERFUND; An ENERgy Retroit FUNding rating tool  
Peter Bevk, B. Sc.  
European Commission
4. H2020 - ODYSSEE-MURE; ODYSSEE-MURE, A Decision Support Tool for Energy Efficiency Policy Evaluation  
Dr. Fouad Al-Mansour  
European Commission
5. H2020 - guarantEE; Energy Efficiency with Performance Guarantees in Private and Public Sector  
Damir Staničič, M. Sc.  
European Commission

## RESEARCH PROGRAM

1. Modelling and environmental impact assessment of processes and energy technologies  
Dr. Fouad Al-Mansour

## NEW CONTRACTS

1. A supermonitoring of the guarantee measurements of the Flue Gas Desulphurization Plant of unit 6 of the Šoštanj Thermal Power Plant  
Boris Sučić, M. Sc.  
Teš d. o. o.
2. Elaboration of a study of energy system optimization  
Stane Merše, M. Sc.  
Koto d. o. o.
3. Concerted action in the field of the Directive on end energy efficiency (CA ESD II)  
Damir Staničič, M. Sc.  
Ministry for Infrastructure and Spatial Planning
4. 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 for Infrastructure and Spatial Planning
5. Action plan for energy efficiency and reporting on its carrying out  
Damir Staničič, M. Sc.  
Ministry for Infrastructure and Spatial Planning
6. Framework agreement on the professional advising in the field of cogeneration  
Stane Merše, M. Sc.  
Energetika Ljubljana, d. o. o.
7. Updating, Upgrading and Publishing on the Web of Energy and Environment Indicators 2015 and preparation of a framework proposal for the publication Environment and energy in Slovenia  
Matjaž Česen, B. Sc.  
Ministry for Environment and Spatial Planning

8. Strategic Studies for the Revision of the NEC Directive, Questionnaires CLRTAP and Improvement of Emission Inventory  
Matjaž Česen, B. Sc.  
Ministry for Environment and Spatial Planning
9. Inclusion in the procedure of integrated assessment of impacts on the environment for an updated Action plan for RES for the period 2010 – 2020  
Andreja Urbančič, M. Sc.  
Ministry for Infrastructure
10. Preparation of the second two-year report of developed countries for carrying out of the Kyoto Protocol in accordance with relevant conclusions of the Conference of the Parties of the UN Framework Convention on Climate Change  
Andreja Urbančič, M. Sc.  
Ministry for Environment and Spatial Planning
11. Preparation of the tender ELENA for acquiring grants for carrying out Preparation and financing of investments in sustainable energy in littoral municipalities  
Damir Staničič, M. Sc.  
Golea, Nova Gorica
12. Strategic studies for elaboration of a report on measures for the reduction of greenhouse gases emissions and projections of GHG emissions, Second annual report on carrying out of the Operative programme of emissions reduction measures  
Andreja Urbančič, M. Sc.  
Ministry for Environment and Spatial Planning
13. European energy manager IX  
Stane Merše, M. Sc.
14. Energy managers days  
Časnik Finance  
Stane Merše, M. Sc.
15. Refreshment, Upgrading and Publishing on the Web of Energy and Environment Indicators 2015  
ARSO  
Matjaž Česen
16. Energy Consumption of Slovenian Households Based on Model Calculation for 2015  
SURS  
Matjaž Česen
17. Improvement of model data on energy use in transport and impact of transit transport  
MOP  
Matjaž Česen
18. Preparation of strategic studies for elaboration of strategic documents, action plans and measures from the field of energy  
Mzl  
Stane Merše, M. Sc.
19. Elaboration of the concept of space analysis of heat consumption and production for carrying out of the local energy concept of the Municipality of Maribor  
JP Energetika Maribor d.o.o.  
Damir Staničič
20. Study of the natural gas consumption in the Coastal-Karst region  
Plinovodi d.o.o.  
Stane Merše, M. Sc.
21. Elaboration of a concept of introduction of advanced energy services and solutions for industry and local communities based on smart energy grids  
Petrol Energetika Ravne  
Aleš Podgornik, M. Sc.
22. Refreshment, of indicators from the field of Environment and Energy for the needs of the report on Environment for 2017  
MOP  
Matjaž Česen

## STAFF

### Researchers

1. Dr. Fouad Al-Mansour
2. Stane Merše, M. Sc., Head
3. Damir Staničič, M. Sc.
4. Andreja Urbančič, M. Sc.

### Technical officers

5. Matjaž Česen, B. Sc.
6. Jure Čizman, M. Sc.
7. Polona Lah, B. Sc.
8. Marko Pečkaj, B. Sc.

9. Barbara Petelin Visočnik, M. Sc.
10. Aleš Podgornik, M. Sc.
11. Dr. Matevž Pušnik
12. Boris Sučić, M. Sc.

### Technical and administrative staff

13. Peter Bevk, B. Sc.
14. Marko Đorić, B. Sc.
15. Roza Pergarec, B. Sc.
16. Igor Ribič

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Matevž Pušnik, Fouad Al-Mansour, Boris Sučić, Andrej Gubina, "Gap analysis of industrial energy management systems in Slovenia", *Energy (Oxford)*, vol. 108, pp. 41-49, 2016.
2. Boris Sučić, Fouad Al-Mansour, Matevž Pušnik, Tomaž Vuk, "Context sensitive production planning and energy management approach in energy intensive industries", *Energy (Oxford)*, vol. 108, pp. 63-73, 2016.

### PUBLISHED CONFERENCE CONTRIBUTION

1. Viktor Jejčič, Fouad Al-Mansour, Tomaž Poje, "Ogljični odtis sadjarske pridelave", In: *Actual tasks on agricultural engineering: Proceedings of*

*the 44th International symposium on agricultural engineering, Opatija, Croatia, 23rd-26th february 2016*, pp. 447-457.

2. Aleš Podgornik, Boris Sučić, Boštjan Blažič, "Effects of customized consumption feedback on energy efficient behaviour in low-income households", In: *SDEWES 2014, 9th Conference on Sustainable Development of Energy, Water and Environment Systems*, Istanbul-Venice, September 20-27, 2014, *J. Clean. Prod.*, vol. 130, pp. 25-34, 2016.

### MENTORING

1. Matevž Pušnik, *Contextual model of energy use in industry*: doctoral dissertation, Ljubljana, 2016 (mentor Andrej Gubina).
2. Kristijan Lesan, *Recommissioning for more efficient use of energy in non-residential buildings*: master's thesis, Krško, 2016 (mentor Zdravko Praunseis; co-mentor Boris Sučić).

# CENTRE FOR ELECTRON MICROSCOPY AND MICROANALYSIS

# CEMM

*The Centre for Electron Microscopy and Microanalysis (CEMM) is an instrumental centre at the JSI that combines analytical equipment in the field of electron microscopy and microanalysis. Access to the research equipment of the CEMM is provided to other JSI departments as well as other research institutions, universities and industrial partners. The equipment at the CEMM is used by researchers interested in the morphology and the structural and chemical characterization of materials between the micrometre and atomic levels. At the CEMM there are three scanning electron microscopes (JSM-5800, JXA-840A, JSM-7600F), two transmission electron microscopes (JEM-2100 (CO NIN), JEM-2010F) and the equipment for sample preparation. CO NAMASTE contributed to the equipment for electron microscopy with a CCD camera and an ADF detector for the JEM-2010F microscope and an EBSD system for the JSM-7600F. In 2015, the JSI also contributed a GIF spectrometer for the transmission electron microscopy ARM 200CF installed at the KI, and thus became a 20% owner of the entire microscope.*

*Research, involving staff and equipment at CEMM, is diverse regarding the investigated materials and also the used methods. Scanning electron microscopy (SEM) is used to observe the morphology and structure of surfaces and for a microstructural investigation and determination of the chemical composition of polycrystalline oxide and non-oxide ceramic materials, nanostructures, metallic magnetic materials, metals, alloys, glass, etc. All of the scanning electron microscopes in the CEMM are equipped with an energy-dispersion (EDXS) and/or the wavelength dispersion (WDXS) spectrometers of X-rays, allowing a non-destructive determination of the chemical composition of the investigated materials. The scanning electron microscope JSM-7600F is additionally equipped with an electron back-scattered diffraction (EBSD) detector and an electron lithography system.*

*Transmission electron microscopy (TEM) provides an insight into the structure of the material on the nano-scale. Transmission electron microscopy enables structural and chemical analyses of the grain boundaries, planar defects, dislocations and precipitates. The transmission electron microscope JEM-2100 is equipped with an EDXS spectrometer and a CCD camera, and the JEM-2010F is additionally equipped with a STEM unit, EDXS and EELS spectrometers, and a CCD camera. The CEMM also manages the necessary equipment for the SEM and TEM sample preparation.*

The operation of the centre is managed by properly trained employees. Besides maintenance of the equipment, among other CEMM activities are the training of new operators, the organization of workshops and conferences on the topic of electron microscopy, providing services for industrial partners and the introduction of new analytical techniques. CEMM personnel are also responsible for the demonstration of electron microscopy to the general public in the scope of organized visits to the JSI, as well through publications in traditional and digital media. In cooperation with the project "Science on the Street" we successfully completed a "best idea in electron microscopy competition" for the general public. For users of microscopes the CEMM organized the 3rd and 4th workshops (SEM graphical user interface on a JSM-7600F and Microanalysis-EDS). The aim of the workshops was to present the operation of the equipment and microanalysis techniques, especially EDS.

## Some outstanding publications in the past year

1. Journal of materials chemistry. C (Montazer, Amir Hassan, Ramazani, Abdolali, Almasi Kashi, Mohamad, Zavašnik, Janez. Angular-dependent magnetism in Co(001) single-crystal nanowires : capturing the vortex nucleation fields)
2. Sensors and actuators. B, Chemical, (Stanković, Dalibor M., Mehmeti, Eda, Zavašnik, Janez, Kalcher, Kurt. Determination of nitrite in tap water : a comparative study between cerium, titanium and selenium dioxide doped reduced graphene oxide modified glassy carbon electrodes)
3. Journal of physics (Montazer, Amir Hassan, Ramazani, Abdolali, Almasi Kashi, Mohammad, Zavašnik, Janez. Developing high coercivity in large diameter cobalt nanowire arrays.)



Head:  
Prof. Miran Čeh

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**In 2016 the CEMM collaborated with institutions and researchers from the following countries: Croatia, Serbia, Austria, Greece, Portugal, Finland and Iran.**

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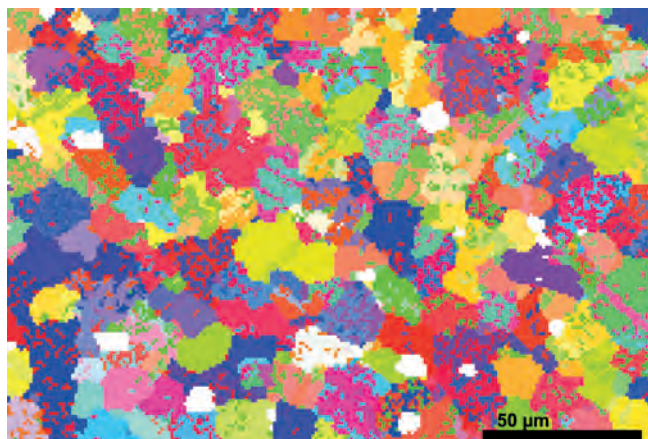


Figure 1: EBSD image of grains in a  $\text{BiFeO}_3$  thick film (published in: *ACS Appl. Mater. Interfaces* 2016, 8, 19626–19634, "Self-Poling of  $\text{BiFeO}_3$  Thick Films", DOI: 10.1021/acsami.6b05885) (Evgeniya Khomyakova, K5, Jeol JSM-7600F)

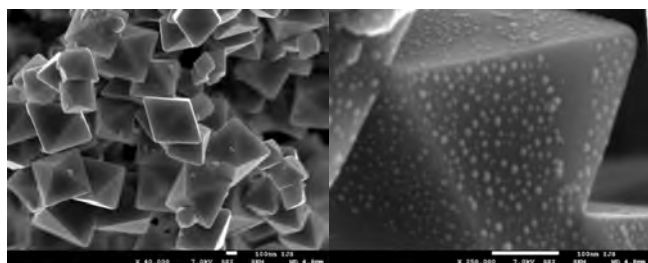


Figure 3: FESEM images of  $\text{In}_2\text{O}_3$  octahedrons decorated with Pt nanoparticles; at lower (left) and higher (right) magnification. Material was synthesized by the AACVD (ang. aerosol assisted chemical vapour deposition) technique. Results were published in S. Roso, C. Büttencourt, P. Umek, O. González, Frank Güell, A. Urakawa and E. Llobet, *Journal of Materials Chemistry C* (2016), 4, 9418–9425.

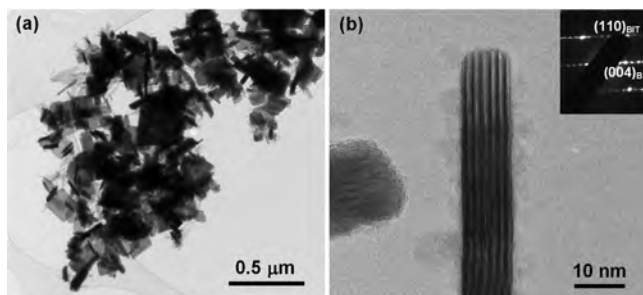


Figure 2: Transmission electron microscopy (TEM) image (a) shows ferroelectric bismuth titanate (BIT) platelets. A high-resolution image with the corresponding electron-diffraction pattern (b) shows a coating of amorphous iron-oxihydroxide nanoparticles deposited at the BIT platelet (author: Blaž Belec).

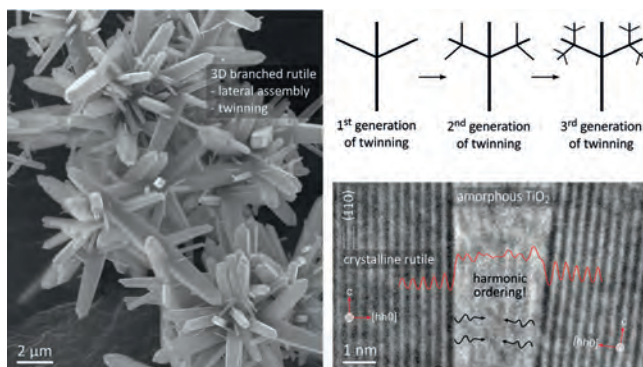


Figure 4: Multilevel branched  $\text{TiO}_2$  structures were shown to be a result of mesocrystal assembly of precipitated rutile fibers that are attached exclusively by low-energy  $\{110\}$  and  $\{101\}$  planes. Harmonic ordering of amorphous material encapsured in intercrystal pores indicates the presence of force-fields that are responsible for oriented attachment of crystals. *Scientific Reports*, DOI: 10.1038/srep24216 (Vanja Jordan, K7, Jeol JSM-7600F & JSM-2100).

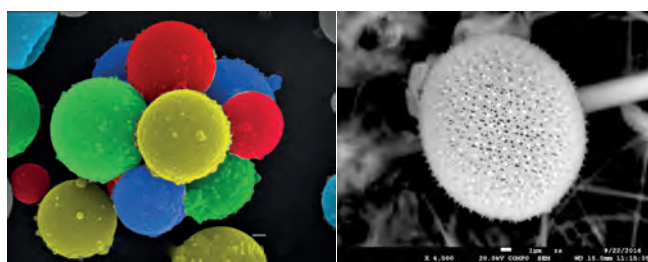


Figure 5: Microcapsule (left) and spherical microporous silicate structure from the river Pesnica suspended matter (right). Published in Kanduč, Tjaša, Samardžija, Zoran, Mori, Nataša, Jerebic, Andreja, Levačič, Ines, Kračun, Miha, Robinson, Johanna A., Žigon, Stojan, Blažeka, Željko, Kocman, David. *Hydrogeochemical and isotopic characterization of Pesnica River, Slovenia = Hidrogeokemične in izotopske značilnosti reke Pesnice. Geologija*, ISSN 0016-7789. 2016, vol. 59, št. 2, str. 179-192. (Dr. Zoran Samardžija, K7, Jeol JXA-840 & JSM-7600F).

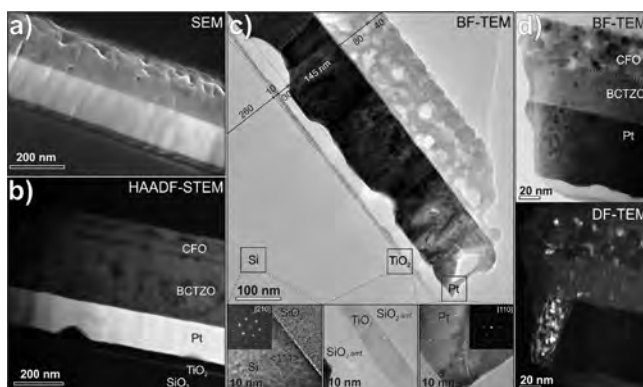


Figure 6: CFO-BCTZO thin-film characterization. *J. Appl. Phys.* doi: 10.1063/1.4961394; CEMM, Jeol S/TEM JEM-2010F

## INTERNATIONAL PROJECT

- Education-ED-FU, EUROFUSION  
Andreja Šestan, B. Sc.

## NEW CONTRACT

- Compatibility assessment between chosen primary wrapper and biological drug  
Prof. Miran Čeh

## STAFF

## Researcher

1. Prof. Miran Čeh, Head

## Postdoctoral associates

2. Dr. Jitka Hreščak

3. Dr. Janez Zavašnik

## Postgraduates

4. Andreja Šestan, B. Sc.

## Technical officers

5. Maja Koblar, B. Sc.

## BIBLIOGRAPHY

## ORIGINAL ARTICLE

1. Nevena Čelić, Egon Pavlica, Miloš Borovšak, Jure Strle, Jože Buh, Janez Zavašnik, Gvido Bratina, Patrick Denk, Markus Scharber, Niyazi Serdar Sariciftic, Dragan Mihailović, "Factors determining large observed increases in power conversion efficiency of P3HT:PCBM solar cells embedded with  $\text{Mo}_6\text{S}_9\text{-xI}_x$  nanowire", *Synth. met.*, vol. 212, pp. 105-112, 2016.
2. Marja Jerič, Johannes de Boor, Janez Zavašnik, Miran Čeh, "Lowering the thermal conductivity of  $\text{Sr}(\text{Ti}_{0.8}\text{Nb}_{0.2})\text{O}_3$  by SrO and CaO doping emicrostructure and thermoelectric properties: microstructure and thermoelectric properties", *J. Mater. Sci.*, vol. 51, no. 16, pp. 7660-7668, 2016.
3. Luka Kelhar, Janez Zavašnik, Paul J. McGuinness, Spomenka Kobe, "The impact of processing parameters on the properties of Zn-bonded Nd-Fe-B magnet", *J. magn. magn. mater.*, vol. 419, pp. 171-175, 2016.
4. Amir Hassan Montazer, Abdolali Ramazani, Mohammad Almasi Kashi, Janez Zavašnik, "Angular-dependent magnetism in Co(001) single-crystal nanowires: capturing the vortex nucleation fields", *J. mater. chem. C*, vol. 4, no. 45, pp. 10664-10674, 2016.
5. Amir Hassan Montazer, Abdolali Ramazani, Mohammad Almasi Kashi, Janez Zavašnik, "Developing high coercivity in large diameter cobalt nanowire arrays", *J. phys., D, Appl. phys.*, vol. 49, no. 44, pp. 445001-1-445001-14, 2016.
6. Branko Pivac, Pavo Dubček, Jasminka Popović, Jasna Dasović, Sigrid Bernstorff, Nikola Radić, Janez Zavašnik, "Influence of stress on the properties of Ge nanocrystals in an  $\text{SiO}_2$  matrix", *J. Appl. Crystallogr.*, vol. 49, part 6, pp. 1957-1966, 2016.

7. Aleksander Rečnik, Janez Zavašnik, Lei Jin, Andrea Čobić, Nina Daneu, "On the origin of "iron-cross" twins of pyrite from Mt. Katarina, Slovenia", *Mineralogical Magazine*, vol. 80, no. 6, pp. 937-948, 2016.
8. Dalibor M. Stanković, Eda Mehmeti, Janez Zavašnik, Kurt Kalcher, "Determination of nitrite in tap water: a comparative study between cerium, titanium and selenium dioxide doped reduced graphene oxide modified glassy carbon electrodes", *Sens. actuators, B, Chem.*, vol. 236, pp. 311-317, 2016.
9. E. Venkata Ramana, Janez Zavašnik, M. P. F. Graça, M. A. Valente, "Magnetoelectric studies on  $\text{CoFe}_2\text{O}_4/0.5(\text{BaTi}_{0.8}\text{Zr}_{0.2}\text{O}_3) - 0.5(\text{Ba}_{0.7}\text{Ca}_{0.3}\text{TiO}_3)$  lead-free bilayer thin films derived by the chemical solution deposition", *J. appl. phys.*, vol. 120, no. 7, pp. 074108-1-074108-10, 2016.

## PUBLISHED CONFERENCE CONTRIBUTION

1. Janez Zavašnik, "Pyrite - pyrrhotite intergrowths in calcite marble from Bistriški Vintgar, Slovenia", In: *Proceedings of the 14th European Workshop on Modern Developments and Applications in Microbeam Analysis (EMAS 2015)*, Portorož, (IOP conference series, Materials science and engineering, Vol. 109), pp. 012020-1-012020-7, 2016.

## PH. D. THESIS

1. Jitka Hreščak, *Synthesis and characterization of undoped and strontium-doped potassium sodium niobate ceramics*: doctoral dissertation, Ljubljana, 2016 (mentor Andreja Benčan Golob; co-mentor Barbara Malič).



# 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.*



Head:  
**Mitja Jermol, M. Sc.**

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 2016 the centre was active in several European projects from FP7: NRG4CAST (Energy Forecasting), 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), SUNSEED (Sustainable and Robust Networking), FI-IMPACT (Future Internet Impact), and some projects from H2020 program: EDSA (European Data Science Academ), AQUASMART (Aquaculture Smart and Open Data Analytics as a Service), OPTIMUM (Multi-source Big Data Fusion Driven Proactivity for Intelligent Mobility) and MOVING (TraininG towards a society of data-saVvy inforMation prOfessionals to enable open leadership Innovation)

In 2016 the centre was active in 10 European projects. The centre prepares and organizes educational events, such as: conferences, seminars, workshops, and summer schools. They are targeted at experts who would like to apply the latest knowledge and achievements from intelligent data analysis, knowledge technologies, data mining, text mining and decision support to the areas of network organizations, business decisions, finance, marketing, automatization and process control. A special consideration is put on the managers and decision makers who are aware of the strengths and benefits to the success of their business. All educational events are designed to transfer basic, additional and 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 22,561 recorded tutorials from different scientific events and it was visited by 744,027 different 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, it is a way of opening up education to everyone for everyone as there is a great need to share educational content on all levels in order to benefit society and foster economy. It also gives a learning opportunity to audiences of all social levels.

VideoLectures.Net has strong connections to the Open Cast Foundation, Open Course Ware Consortium and Knowledge 4 All Foundation Ltd.

In 2016 we organized the 11th Student Competition in Computer Science, attended by 202 students from Slovenian secondary schools. We have also organized project meetings for different EU projects (Xlime, EDSA), coorganized LREC - 10th edition of the Language Resources and Evaluation Conference attended by more than 1000 experts from linguistic field and ESWC "Extended Semantic Web Conference" Summer School, held in Dubrovnik in Croatia.

Within the UNESCO Chair (<http://unesco.ijs.si/>), we attended several international meetings of experts on open education and free educational resources. In March 2016 we represented our achievements at the annual informal meeting of the European Network of National Commissions for UNESCO, held in Krakow at Poland.

The UNESCO chair also participated in the publication of the "Making Sense of MOOCs: A Guide to Policy Makers and Developing Countries". Most of the work based on the preparations for the the 2nd World Open Educational Resources (OER) Congress and participation in the Advisory Group for the preparation of "Slovenian package promotion" in the field of OER, which will be presented at the Congress. The Congress will be held in September 2017 in Ljubljana. The Chair is also included in the advisory committee for the regional consultations conducted by the Commonwealth of Learning, which will be held in six regions of the world. The results will be presented at the 2nd World Congress in Ljubljana.

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**In 2016 the Centre for Knowledge Transfer in IT was actively involved in 10 European projects.**

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**CT3 operates the web portal <http://videlectures.net/>, which is now the biggest world reference portal presenting high-quality scientific lectures.**

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**In 2016 we finished the second cycle of the My Machine project where 10 prototypes of child dream machines were presented.**

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In June 2016 we completed the second cycle of the My Machine project. The final exhibition was organized in "Ramp Lab" in Ljubljana. There were 10 prototypes of child dream machines that we have achieved together with teachers, pupils, students, and professors from 27 different educational institutions. Our activities in the past year included the preparation of the interim exhibition in January 2016, where the students and pupils – creators of

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**Within the UNESCO Chair (<http://unesco.ijs.si/>), we attended several international meetings of experts on open education and free educational resources.**

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the dream machine – met to exchange ideas, proposals and plans for the implementation of prototypes. In October 2016, we launched the third cycle of the project. This time we collaborate with 12 educational institutions from Ljubljana, Škofja Loka and Velenje. The cycle will be completed in June 2017. More information about that project is available on <http://www.mymachineglobal.org/tag/slovenia/>.

## Organization of conferences, congresses and meetings

1. 11th Student competition in computer science, Ljubljana, 19. 3. 2016
2. Project meeting of the EU project Xlime, Dubrovnik, Croatia, 16.-18. 5. 2016
3. Coorganization of the LREC conference, Portorož, Slovenia, 23.-28. 5. 2016
4. Final My Machine Exhibition, Ljubljana, 16. 6. 2016
5. Project meeting of the EU project EDSA, Dubrovnik, Croatia, 23.-24. 6. 2016
6. Coorganization of the ESWC "Extended Semantic Web Conference" Summer School, Dubrovnik, Croatia, 5.-10. 9. 2016

## INTERNATIONAL PROJECTS

1. European Language Resource Coordination (ELRC) 2015, 08.12.2015, JSI, Ljubljana  
Mitja Jermol, M. Sc.  
Dfki Gmbh - Deutsches Forschungszentrum Fuer
2. 7FP - ProaSense; The Proactive Sensing Enterprise  
Mitja Jermol, M. Sc.  
European Commission
3. 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
4. 7FP - xLiMe; CrossLingual CrossMedia Knowledge Extraction  
Mitja Jermol, M. Sc.  
European Commission
5. 7FP - SUNSEED; Sustainable and Robust Networking for Smart Electricity Distribution  
Mitja Jermol, M. Sc.  
European Commission
6. 7FP - FI-IMPACT; Future Internet Impact Assurance  
Mitja Jermol, M. Sc.  
European Commission

7. H2020 - EDSA; European Data Science Academy  
Mitja Jermol, M. Sc.  
European Commission
8. H2020 - OPTIMUM; Multi-source Big Data Fusion Driven Proactivity for Intelligent Mobility  
Dr. Matej Kovačič  
European Commission
9. H2020 - MOVING; Training Towards a Society of Data-Savvy Information Professionals to enable Open Leadership Innovation  
Gaber Cerle  
European Commission

## R&D GRANTS AND CONTRACTS

1. Videorecording and Post-Processing  
Mitja Jermol, M. Sc.
2. My Machine Slovenia  
Mitja Jermol, M. Sc.

## STAFF

### Postgraduates

1. *Dr. Katja Berčič, left 01.07.16*
2. Anja Polajnar, B. Sc.

### Technical officers

3. Mitja Jermol, M. Sc., Head
4. Dr. Matej Kovačič
5. *Marjana Plukavec\*, B. Sc., left 01.04.16*
6. Špela Sitar, B. Sc.

### Technical and administrative staff

7. Aleš Buh

8. Gaber Cerle, B. Sc.
9. Mihajela Črnko
10. Ana Fabjan, B. Sc.
11. Adis Krečo, B. Sc.
12. Monika Kropelj, B. Sc.
13. Davor Orlić, B. Sc.
14. Tanja Zdolšek Draksler, B. Sc.

Note:

\* part-time JSI member

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Mario Karlovčec, Dunja Mladenić, Marko Grobelnik, Mitja Jermol, "Conceptualization of science using collaboration and competences", *Electron. libr.*, vol. 34, no. 1, pp. 2-23, 2016.

### PUBLISHED CONFERENCE CONTRIBUTION

1. Ruben Costa, Ricardo Jardim-Gonçalves, Paulo Figueiras, Margherita Forcolin, Mitja Jermol, Richards Stevens, "Smart cargo for multimodal freight transport: when "cloud" becomes "fog"", In: *8th IFAC Conference on Manufacturing Modelling, Management and Control MIM 2016, Troyes, France, 28-30 June 2016, IFAC-PapersOnline*, vol. 49, no. 12, pp. 121-126, 2016.

# MILAN ČOPIČ NUCLEAR TRAINING CENTRE

## ICJT

*The mission of the training centre ICJT is training in the field of nuclear technologies and radiation protection. In addition, ICJT is actively informing the public about those technologies.*

Training in the area of nuclear technologies is our primary mission. In the autumn of 2016, the 37<sup>th</sup> course *Basics of Nuclear Technology* was conducted. The participants were mainly from the Slovenian Nuclear Safety Administration (SNSA) and there were also two participants from Krško NPP and two participants from technical support organizations. In parallel, the 16<sup>th</sup> edition of course *Nuclear Technology* started. This course is the initial theoretical training of future nuclear-power-plant control-room operators and is normally organized every second year.

There were 29 radiological protection training courses for medical, industrial and research use of radioactive sources.

In collaboration with the reactor physics division, we organized an international course in the area of regulatory control of research reactors.

Public information remains an important part of our activities. Groups of visitors (mainly schoolchildren, students and various societies) were regularly attending the lectures and visiting the permanent exhibition on nuclear energy, smaller groups the TRIGA reactor and/or the accelerator. In addition to traditional lectures on electricity from nuclear energy, radioactive waste or fusion, we have prepared two new lectures for general public, an energy workshop and a lecture on isotopes. Altogether, there were 161 groups or 6825 visitors this year. Since 1993, a total of 168,644 pupils, teachers and others, visited our information centre. We have continued monitoring and analysing media reports on nuclear energy.



Head:  
**Dr. Igor Jenčič**

**In 2016 we prepared two new lectures for general public: an energy workshop, suitable for junior elementary school pupils, and a lecture on isotopes that is focused on the uses of analysing stable isotopes.**



Figure 1: IJS Open day at the Nuclear Training Centre



Figure 2: Energy Workshop at the Elementary School Hotič



Figure 3: Basics of Nuclear Power Plant Technology Course (radioactivity workshop)



Figure 4: Training Course on Requirements and safety evaluation of Research Reactors (EC INSC Project MC3.01/13), December 2016

## Table of training activities at the Nuclear Training Centre in 2016

Date	Title of the course	Parti- pants	Lecturers	Weeks	Participants × weeks
25. - 29.1.	Radiation protection for RP department staff - Refresher course	13	6	1	13
10.2.	Radiation protection for industrial and other practices	11	2	0.2	2.2
17.2.	Radiation protection for industrial and other practices	10	2	0.2	2
25. - 26.2.	Radiation protection for Dental Radiography	4	3	0.2	0.8
7. - 10.3.	Radiation protection for Dental Radiography	1	5	0.4	0.4
7. - 9.3.	Radiation protection for industrial and other practices (unsealed sources)	3	4	0.6	1.8
7. - 9.3.	Radiation protection for industrial and other practices (sealed sources)	9	4	0.6	5.4
7. - 9.3.	Radiation protection for workers exposed to radon and thoron	1	5	0.6	0.6
15.3.	Radiation protection for industrial and other practices (sealed sources) - Refresher Course	27	4	0.2	5.4
15.3.	Radiation protection for industrial and other practices (measurement of road-way density and humidity) - Refresher Course	3	4	0.2	0.6
15.3.	Radiation protection for industrial and other practices (radiography) - Refresher Course	6	4	0.2	1.2
17.3.	Training Extension for RP Officers	1	2	0.2	0.2
17.3.	Training Extension for RP Officers	15	2	0.2	3
18.3.	Radiation protection for Dental Radiography - Refresher Course	11	4	0.2	2.2
18.3.	Radiation protection for exposed workers in medicine and veterinary - Refresher Course	1	4	0.2	0.2
21. - 23.3.	Radiation protection for medical and veterinary workers - radiological diagnostic	1	4	0.6	0.6
21. - 23.3.	Radiation protection for medical and veterinary workers	2	4	0.6	1.2
5.4.	Radiation protection for industrial and other practices (min. exposed workers)	17	3	0.2	3.4
6. - 10.6.	Radiation protection for exposed workers in Krško Nuclear Power Plant	11	7	1	11
10. - 14.10.	Radiation protection for medical and veterinary workers - Nuclear medicine workers	2	9	1	2
10. - 12.10.	Radiation protection for industrial and other practices (sealed sources)	9	4	0.6	5.4
10. - 13.10.	Radiation protection for Dental Radiography	2	5	0.4	0.8
18.10.	Radiation protection for industrial and other practices (sealed sources) - Refresher Course	19	4	0.2	3.8
18.10.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	2	5	0.2	0.4
18.10.	Radiation protection for industrial and other practices (measurement of road-way density and humidity) - Refresher Course	1	4	0.2	0.2
20.10.	Training Extension for RP Officers	7	2	0.2	1.4
20.10.	Training Extension for RP Officers	1	0	0.2	0.2
21.10.	Radiation protection for Dental Radiography - Refresher Course	9	3	0.2	1.8
2. - 30.11.	Basics of nuclear technology, theory	11	13	4.2	46.2
14.11 - (14.4.2017)	Nuclear Technology, Theory	5	23	21.6	108

## Table of training activities at the Nuclear Training Centre in 2016

Date	Title of the course	Parti- pants	Lecturers	Weeks	Participants × weeks
1. - 23.12.	Basics of nuclear technology, systems	10	10	3.4	34
5. - 9.12.	EU Dedicated Training Course on "Requirements and safety evaluation of Research Reactors"	11	9	1	11
19.12.	Radiation protection for exposed workers in medicine and veterinary - Refresher Course	1	2	0.2	0.2
<b>TOTAL</b>		<b>237</b>	<b>166</b>	<b>41.2</b>	<b>270.6</b>

## INTERNATIONAL PROJECTS

- 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
- Training and Tutoring for Experts of the National Regulatory Authorities and their Technical Support Organisations for Developing or Strengthening their Regulatory and Technical Capabilities - MC3.01/13  
Saša Bobič  
Iter-consult Srl - Independent

- Trainings of the Radiation protection  
Matejka Južnik, M. Sc.

## NEW CONTRACTS

- Public information and monitoring of media regarding nuclear energy and activities of GEN-energija  
Dr. Igor Jenčič  
Gen Energija, d. o. o.
- ICJT Training Programme implementation in the year 2016 and 2017  
Dr. Igor Jenčič  
Nuklearna Elektrarna Krško
- Basic Training Course on Nuclear Technology and Nuclear Power Plants  
Dr. Igor Jenčič  
Ministrstvo za okolje in prostor

## R & D GRANTS AND CONTRACTS

- Trainings of the RP for Foreign Market  
Matejka Južnik, M. Sc.

## STAFF

### Researcher

- Dr. Igor Jenčič, Head

### Technical officers

- Jure Hribar, B. Sc.
- Rado Istenič, B. Sc., retired 01.08.16
- Matjaž Koželj, M. Sc.
- Tomaž Skobe, M. Sc.

- Vesna Slapar Borišek, B. Sc.

- Luka Tavčar, B. Sc.

- Nina Udir, B. Sc., 01.06.16, transferred to Department SVPIŠ

### Technical and administrative staff

- Saša Bobič
- Matejka Južnik, M. Sc.
- Borut Mavec, B. Sc.

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

- Matjaž Koželj, Bruno Cvikel, "The negative mobility: An outcome of the electric field at the hole-injecting metal/organic semiconductor interface that varies as a linear function of the applied bias", *Thin solid films*, vol. 616, str. 786-792, 2016.

### PUBLISHED CONFERENCE CONTRIBUTION

- Radko Istenič, Igor Jenčič, "Public Opinion about Nuclear Energy - Year 2016 Poll", In: *Proceedings*, 25th International Conference Nuclear Energy for New Europe - NENE 2016, Portorož, Slovenia, September 5-8, 2016, 8 pp.
- Igor Jenčič, "The use of Ljubljana TRIGA reactor in training of NPP operators and public information", In: *2016 ANS Winter Meeting and Nuclear Technology Expo*, November 6-10, 2016, Las Vegas, *Transactions of ANS*, vol. 115, p. 92, 2016.

- Igor Jenčič, Luka Snoj, "The use of Ljubljana TRIGA reactor for training and public information", In: *Role of research reactors in providing support to nuclear power programmes*, Report of the IAEA Technical Meeting on "Role of Research Reactors in providing support to Nuclear Power Programmes", 21-24 June 2016, Vienna, p. 44.
- Tomaž Skobe, Matjaž Leskovar, "Material influence on ex-vessel steam explosion", In: *Proceedings*, 25th International Conference Nuclear Energy for New Europe - NENE 2016, Portorož, Slovenia, September 5-8, 2016, pp. 813-1-813-10.
- Vesna Slapar Borišek, "Energy for children", In: *Proceedings*, 25th International Conference Nuclear Energy for New Europe - NENE 2016, Portorož, Slovenia, September 5-8, 2016, 6 pp.

### MASTER'S THESIS

- Tomaž Skobe, *Analysis of steam explosion in flooded reactor cavity*: master's thesis, Ljubljana, 2016 (mentor Matjaž Leskovar).



# RADIATION PROTECTION UNIT

# SVPIS

*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 one 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 using an accredited method (EN ISO/IEC 17025).*

## Personal dosimetry

The personal doses of 126 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters. The maximum individual yearly dose was 0.21 mSv. This is only 1 % of the regulatory limit for occupational exposure (20 mSv per year) and 21 % of the limit for the general public (1 mSv per year). The collective dose at the JSI in 2016 was 1.5 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 2016 19 inspections in other JSI laboratories were performed. 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, 112 sources of radiation are used, which require regulatory control. Additionally, 4443 low-activity sources are also used in different laboratories.

## Environmental monitoring

The environmental monitoring of the Reactor Center was performed according to 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 2016 due to activities at the Reactor Center was insignificant.**

## Expert assessments and measurements for outside customers

The Radiation Protection Unit is authorized to supervise measurements and conduct expert assessments in the field of radiation protection. In the past year several radiological control investigations were carried out in industrial and research institutions. Our group has participated in an evaluation of the radiological monitoring of Krško NPP, research reactor TRIGA and storage for low- and intermediate-level waste in Brinje.



Head:

**Matjaž Stepišnik, M. Sc.**

## STAFF

### Technical officer

1. Dr. Tinkara Bučar
2. Matjaž Stepišnik, M. Sc., Head

### Technical and administrative staff

3. Emira Bašić, B. Sc.
4. Thomas Breznik, B. Sc.
5. Nina Udir, B. Sc.

## BIBLIOGRAPHY

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### PUBLISHED CONFERENCE CONTRIBUTION

1. Michel Cindro, Matjaž Stepišnik, Damir Pinezić, Davor Sinka, Dejan Skanata, "Physical and radiological characterisation of measuring sites within the Croatian gamma dose rate early warning network", In: *Conference proceedings and book of abstracts: former "Nuclear Option in Countries with Small and Medium Electricity Grids"*, 11th International Conference of the Croatian Nuclear Society, June 05-08, 2016, Zadar, Croatia, pp. 113-1-113-15.

### INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Matjaž Stepišnik, "Reka Sava", In: *Ovrednotenje izpustov iz NEK in primerjava z meritvami v okolju*, Matjaž Stepišnik, et al, 1. izd., Ljubljana, Institut Jožef Stefan, 2016, pp. 1-20.

# CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION CTT

*In 1996 the Office of Technology Transfer was established and – based on its work – since January 2011 an independent Center for Technology Transfer and Innovation (CTT) continues its mission at the Jožef Stefan Institute. We assist in the process of technology and knowledge transfer from the JSI to the economy, which includes licensing, spin-out creation, associated procedures for the protection of intellectual property and assisting companies with finding suitable local and international research partners for contract and collaborative research. We also transfer knowledge from science to the school system and promote the recognisability of the JSI and science in general among young people and the wider population.*



Head:  
**Dr. Špela Stres, MBA, LL.M.**

The center's success is based on the work of 9 professionals, 5 of which are educated in natural sciences and engineering, 4 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 Science and Technology Professionals), the LES (Licensing Executives Professionals) and we hold the U. S. certificate "Certified Licensing Professional".

An important tool in our work is the networks of contacts successfully created with enterprises and other organisations in Slovenia and abroad. Our services, fine-tuned towards individual needs, are offered to JSI researchers and external organisations and include first meeting, needs analysis, registration and protection of intellectual property, marketing of intellectual property (including secret know-how), negotiations and the preparation of suitable agreements. The part of financial means is contributed by researchers of the JSI through their commission, while our direct clients in 2016 were represented by numerous companies and other research organisations.

In 2016 the CTT was partly funded through five larger and numerous smaller EU and national projects. These projects belonged to various funding programmes and schemes: Openisimes (CIP scheme), Enterprise Europe Network Slovenia (CIP scheme), We4SMESLO (Horizon 2020) and two projects connected to science in school system: SciChallenge (Horizon 2020) and STEM4YOUTH (Horizon 2020). Project activities were connecting and completing our core TT activities.

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 (36 cases), gives first advice to researchers (27), prepares assessments of patentability – reviews state of the art (12). The number of these activities has risen considerably in comparison with previous years. The group also evaluates market potential, helps prepare the invention for disclosure within the research organisation, helps draft the patent applications, prepares agreements on the ownership of intellectual property, advises on the choice of patent attorney, prepares and files the patent application and gives advice about the strategy of the international (3) and national expansion of patent protection. The group also takes care of the active marketing of technologies IJS (7 technologies promoted to 250 enterprises and other organisations, 12 technologies promoted on global base Enterprise Europe Network). It manages received interests and starts the negotiations (16). Moreover, group members arrange for the signing of non-disclosure agreements (19), manage affairs with partners in different consortia (5), take part in negotiations (16), prepare license agreements (3) and arrange their signature. Experts that belong to this group provide individual consulting regarding all the phases of spin-out company formation, help with the preparation of business plans, manage discussions on the arrangement of the relationship between JSI and the researcher and prepare license agreements for the use of technology within the spin-out company. To encourage the researches in their entrepreneurial aspirations, this group's experts organize a contest for the selection of innovations with the highest commercial potential and various workshops for young researches. In 2016 one spin-out company was created, two cases were in the final stages.

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**Marketing of 15 JSI technologies, procedures for the creation of spin-out companies, 40 identified RR topics.**

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**Organisation of two visiting groups BioChem-Tech and Materials, composed of experts in the field of technology transfer.**

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**Organisation of 9<sup>th</sup> International Technology Transfer Conference – more than 125 visitors, competition for best innovation idea, international visit from Slovenia, EU countries and China, 68 B2R meetings.**

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The above-mentioned group closely cooperates with the **Group for contractual collaboration with economy**, which visits both large (45 since 2012) and small companies (18 in 2016), organises their return visits to the JSI, organises sector and regional visits of companies to the JSI and collaborates with other support environment entities. This group's members are trying to find new topics for cooperation within the development projects amongst companies and researches (40), prepare technology offers, arrange for the signing of non-disclosure agreements and acquire written consent for further cooperation (14). The group also takes part in various events; in the course

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**4000 visitors during the Open Day at JSI,  
83 school visits.**

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of the 9th International Technology Transfer Conference it organised individual meetings between companies and researchers (63). In 2016 we hosted two sector groups, which function within the Enterprise Europe Network, namely sector group Materials and sector group BioChemTech (altogether 39 foreign visitors). In the course of the visit the members of sector groups met 11 Slovenian companies and visited 7 JSI departments. CTT has actively promoted some spin-out companies of JSI (4), for which 5 different potential partners are currently interested.

**Group for promotion, education and project management** has prepared and disseminated lists of Slovenian and EU tenders (12) and foreign partner searchers, helped prepare project applications, especially in the Exploitation and Dissemination parts, weekly disseminated other information to TT coordinators, which has efficiently contributed to the application of new projects with foreign partners (13). The group has successfully spread various information through the CTT e-newsletter and CTT's Facebook profile, organised Open Day at the JSI (4000 visitors, which is almost 3 times more than the previous year), organised 83 school visits at the JSI (with an additional 3160 visitors), provided entrepreneurial education to young researchers in compliance with Slovenian Research Agency's requirements (25 participants), and organised the 9th International Technology Transfer Conference (125 participants, one-third of them from abroad).

**Group for research in the field of technology transfer and innovation** has participated in two studies of the Europe Commission Advisory Group for Future and Emerging technologies; it has participated in the realization of the first boot camp in the field of technology transfer at EU level, which was supported by our own lecturers. We have given lectures on our experience with cohesion funds in Brussels, Prague etc. As members of Europe Commission Advisory group for Science with and for Society we helped designing criteria for the evaluation of respective science for further calls. In the frame of the EU support system for progressive technology transfer offices called Progress-TT we develop additional services; we work as evaluators and external experts in the frame of European Commission for different international institutions (Academy of Science Finland; Federal Ministry of

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**2 studies for European Commission. Progress-TT program for progressive technology transfer offices in EU. Some of best-rated commercialization experts of European Commission.**

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Science, Research and Economics, Austria; Investment Fund South East Europe). We have participated in the working group DG Grow, Enterprise Europe Network, which has made recommendations to the European Commission and members of the Enterprise Europe Network about how to implement specialized support services to help companies that are undergoing rapid growth or are entering this phase. As one of the best-rated commercialization external experts in the EU we work for the European Commission and advise different consortia within H2020, with the emphasis on program Industrial Leadership (FoF, NMP, ICT).

## Organization of Conferences, Congresses and Meetings

1. 9th International Technology Transfer Conference, Brdo pri Kranju, 21. September 2016
2. Mladi upi 2016, Education for young researchers, NLB, Ljubljana, 30. May 2016
3. The open-house day, JSI, Ljubljana, 19. March 2016

## INTERNATIONAL PROJECTS

- |   |   |
|---|---|
| <ol style="list-style-type: none"> <li>1. STPII - Second Science and Technology Project - Preparation of Feasibility Studies with Cost Benefit Analysis for Three RDI Infrastructure Projects<br/>Dr. Špela Stres<br/>Wyg Savjetovanje d. o. o.</li> <li>2. OPENiSME; Open Platform for Innovative SMEs; EACI, CIP Programme<br/>Dr. Špela Stres<br/>European Commission</li> <li>3. COSME - EEN Slovenia; EEN Slovenia Services in Support of Business and Innovation in Slovenia<br/>Dr. Špela Stres<br/>European Commission</li> <li>4. H2020 - SCICHALLENGE; Next Generation Science Challenges using Participatory Techniques and Digital Media</li> </ol> | <p>Dr. Špela Stres<br/>European Commission</p> <ol style="list-style-type: none"> <li>5. H2020 - STEM4youth; Promotion of STEM Education by Key Scientific Challenges and their Impact on Our Life and Career Perspectives<br/>Dr. Špela Stres<br/>European Commission</li> <li>6. H2020 - INPRO; Improving IPR Management Service to SMEs Engaging in Peer Learning Activities<br/>Dr. Špela Stres<br/>European Commission</li> <li>7. H2020 - We4SMESLO; Enhancing the Innovation Management Capacity fo SMEs (by EEN), Slovenia<br/>Dr. Špela Stres<br/>European Commission</li> </ol> |
|---|---|

8. H2020 - ReconCell; A Reconfigurable Robot Workcell for Fast Set-up of Automated Assembly Processes in SME-s  
Dr. Špela Stres  
European Commission
9. Promotion of Research Achievements in Applied Projects of the Jožef Stefan Institute on the Autumn Conference ASTP PROTON „Making a Difference through Knowledge Transfer“  
Dr. Špela Stres  
Slovenian Research Agency

## VISITORS FROM ABROAD

1. Tony Raven, Chief Executive, Cambridge Enterprise Limited, University of Cambridge, Cambridge, United Kingdom, 21. September 2016
2. Henric Rhedin, School of Business, Economics and Law, University of Gothenburg, Gothenburg, Sweden, 21. September 2016
3. Jean-Pierre Nozieres, eVaderis, Grenoble, France
4. Silvi Serreqi, EASME, Bruselj, Belgium, 21. September 2016
5. Sergej Paveliev, Zenit Zentrum Fur Innovation Und Technik In Nordrhein-Westfalen Gmbh, Mulheim An der ruhr, Germany, 20.-21. September 2016
6. Wojciech Szmít, Podlaska Fundacja Rozwoju Regionalnego, Lomza, Poland, 20.-21. September 2016
7. Can Kartoglu, Sabanci Universitesi, Istanbul, Turkey, 20.-21. September 2016
8. Tomasz Charkot, Dolnoslaska Agencja Rozwoju Regionalnego Sa, Szczawno-Zdroj, Poland 20.-21. September 2016
9. Ondrej Petrasek, Jic, Zajmove Sdruzeni Pravnickch Osob, Brno -Medlanky, Czech Republic, 20.-21. September 2016
10. Aleksandar Sedmak, Inovacioni Centar Masinskog Fakulteta Doo, Beograd, Serbia, 20.-21. September 2016
11. Sara Maiez-Tribut, Agence Regionale Du Developpement De L'innovation Ardi Rhone-Alpes, Lyon, France, 20.-21. September 2016
12. Jędrzej Danilewicz, Uniwersytet Zielonogorski, Zielona Gora, Poland, 20.-21. September 2016
13. Dries Stoel, Kamer Van Koophandel, Amsterdam, Netherlands, 20.-21. September 2016
14. Tomasz Lyzwinski, Zachodniopomorski Uniwersytet Technologiczny W Szczecinie, Szczecin, Poland, 20.-21. September 2016
15. Aneta Aleksander, Gornoslaska Agencja Przedsiębiorczosci I Rozwoju Sp Zoo, Gliwice, Poland, 20.-21. September 2016
16. Nicole Okoye, Gottfried Wilhelm Leibniz Universitaet Hannover, Hannover, Germany, 20.-21. September 2016
17. Pero von Strasser, Stiftung Fachhochschule Osnabrueck, Osnabrück, Germany, 20.-21. September 2016
18. Elena Cortés Ventura, Red De Institutos Tecnológicos De La Comunidad Valenciana Redit Asociacion, Valencia, Spain, 20.-21. September 2016
19. Emilie MARCELET, Chambre De Commerce Et D'industrie De Region Picardie, Amiens Cedex 1, France, 20.-21. September 2016
20. Olaf Jüptner, Hessen Trade & Invest GmbH, Wiesbaden, Germany, 20.-21. September 2016
21. Elsa Luciani, Agencia Per A La Competitivitat De La Empresa, Barcelona, Spain, 20.-21. September 2016
22. Antonio Cusma, Consiglio Nazionale Delle Ricerche, Rim, Italy, 20.-21. September 2016
23. Andrew Hebb, University Of Greenwich, Chatham, Kent, United Kingdom, 20.-21. September 2016
24. Silvi Serreqi, Executive Agency for Small and Medium Enterprises, Brussels, Belgium, 20.-21. September 2016
25. Magali Parent, Agenschap Voor Innovatie Door Wetenschap En Technologie, Brussels, Belgium, 20.-21. September 2016
26. Stan Francke, Ministerie Van Economische Zaken, Utrecht, Netherlands, 20.-21. September 2016
27. Tim Benzie, University Of Greenwich, Greenwich, United Kingdom, 4.-5.October.2016
28. Sara Di Falco, Regione Piemonte, Piemonte, Italy, 4.-5.October.2016
29. Nunzia Ciliberti, Aster - Societa Consortile Per Azioni, Bologna, Italy, 4.-5.October.2016
30. Claire Melville, Scottish Enterprise, Glasgow, United Kingdom, 4.-5.October.2016
31. Georges De Lacoste, Centre D'accompagnement De Projets Innovants Asbl, Nivelles, Belgium 4.-5.October.2016
32. Isabelle Pottier, Chambre De Commerce Et D'industrie De Region Paris Ile-De-, Paris, France, 4.-5.October.2016
33. Astrid Pauli, Zenit Zentrum Fur Innovation Und Technik In Nordrhein-Westfalen GMBH, Mulheim An der ruhr, Germany, 4.-5.October.2016
34. Bénédicte Ganivet, Chambre De Commerce Et D Industrie De Region Languedoc Roussillon, Perols, France, 4.-5.October.2016
35. Melanie Albrecht, Investitions-Und Förderbank Niedersachsen (NBANK), Hanover, Germany, 4.-5.October.2016
36. Cemile Koseler Usta, Istanbul Sanayi Odasi, Istanbul, Turkey, 4.-5.October.2016
37. Katerina Papadouli, Foundation For Research And Technology Hellas, Athens, Greece, 4.-5.October.2016
38. Frédéric Suche, Agence Bruxelloise Pour L'entreprise, Brussels, Belgium, 4.-5. October.2016
39. Snezana Kirin, Inovacioni Centar Masinskog Fakulteta Doo, Beograd, Serbia, 4.-5. October.2016
40. Leo Donato, Rtc North Limited, Leeds, United Kingdom, 4.-5.October.2016
41. Aleksandar Sedmak, Inovacioni Centar Masinskog Fakulteta Doo, Beograd, Serbia, 4.-5. October.2016
42. dr. Andrea Basso, Progress TT, MITO Technology, Milano, Italy, 5.-6.December. 2016

## STAFF

### Researcher

1. Dr. Špela Stres, MBA, LL.M, Head
- Postdoctoral associates
2. Dr. Asja Grafj, left 05.09.16
  3. Dr. Duško Odić, left 01.05.16
  4. Dr. Levin Pal

### Postgraduates

5. Robert Blatnik, M. Sc.

### Technical officers

6. Lea Aissatou Levpušček, B. Sc.

7. Tomaž Lutman, B. Sc.

8. France Podobnik, B. Sc.

9. Marjeta Trobec, B. Sc.

### Technical and administrative staff

10. Barbara Bercko, B. Sc.

11. Špelca Kompara, B. Sc.

12. Tamara Matevc, B. Sc.

13. Luka Virag, B. Sc.

## BIBLIOGRAPHY

### ORIGINAL ARTICLE

1. Tomas Ekeberg *et al.* (60 authors), "Single-shot diffraction data from the Mimivirus particle using an X-ray free-electron laser", *Scientific data*, vol. 3, pp. 160060-1-160060-7, 2016.

2. Gijs van der Schot *et al.* (44 authors), "Open data set of live cyanobacterial cells imaged using an X-ray laser", *Scientific data*, vol. 3, pp. 160058-1-160058-7, 2016.