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Ljubljana, July 2019

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Milan Čopič Nuclear Training Centre (ICJT)	
Radiation Protection Unit (SVPIS)	
Centre of Technology Transfer and Innovation (CTT)	
Center for Smart Cities and Communities (CSC&C)	
Center Factory of the Future (CFOF)	

## INTRODUCTION

With the end of 2018, the "Jožef Stefan" Institute records 70 years of research activity. Since it was established in 1949, the Institute has evolved and expanded because of the courage and vision of its members and the natural need for high-quality university education based on research. In the 1970s and especially in the 1980s, the Institute began to be influenced by the economy and this led to its rapid growth. After Slovenia gained its independence, this cooperation declined slightly, due mainly to the post-independence crisis of the 1990s and the global economic crisis that occurred in 2008. This most recent event also revealed itself as a crisis of vision in governmental development policies, as Slovenian researchers bore the brunt of tough, uncompromising savings in public expenditure, despite their activities being vitally important for the country's social and economic development.



Nobel laureate Prof. Duncan Haldane (left) during his visit at the Jožef Stefan Institute with director Prof. Jadran Lenarčič

While we in Slovenia were asking ourselves what to do with science and technological development, the smarter countries in Europe maintained a very clear vision. However, let me emphasize, the situation in the country has begun to improve since 2017. Based on the commitments of almost all the political parties in the government and in opposition, it looks like the increasing investments in research and development will continue into the future.



Prof. Oussama Khatib with director Prof. Jadran Lenarčič

During the crisis the Institute became intensively international and sought out opportunities in European exchanges and financial instruments. If anything, it is this international involvement that has shaped our modern Institute. By operating internationally, the institute has excelled in maintaining the number of employees, while strengthening its many international connections, which are the key to success for the future and the drive for quality. In 2018, the Institute ended the year with 991 employees, and it is expected that this number will soon exceed 1000 for the first time in the Institute's history. Lastly, let me repeat that what is most important is that the Institute continues to develop its humane and noble mission, and that it is able to attract and inspire generations of the most talented and creative young people to devote their lives to science and research. These are the historical and cultural dimensions that our Institute has for Slovenia and beyond. In conclusion, I particularly want to thank all those who have left their mark on the Institute.

*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 establish a Physics Institute

#### 1949

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

### 1952

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

#### 1954

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

#### 1956

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

### 1958

 Institute reorganised and new fields of activity defined: nuclear physics, solidstate physics, chemistry, and radiobiology

#### 1959

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



Mass spectrometer at the JSI (about 1960)

### 1962

One of the first compounds of a noble gas, XeF<sub>6</sub>, synthesised at the institute The first computer for research, ZUSE Z23, 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

 $\sim~$  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
- $\sim$   $\;$  Research institutes in Velenje, ERICo and Valdoltra established by the Institute  $\;$
- 1997
- $\sim$  3.5-MeV electrostatic accelerator, TANDETRON, installed

### 1999

~ Jožef Stefan Institute celebrates its 50th 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, Founder and first Director of the Jožef Stefan Institute, 1949–1955 Karol Kajfež, 1955–1958 Lucijan Šinkovec, B. Sc., 1959–1963 Prof. Milan Osredkar, 1963–1975 Prof. Boris Frlec, 1975–1984 Prof. Tomaž Kalin, 1984–1992

Prof. Danilo Zavrtanik, 1992–1996 Prof. Vito Turk, 1996–2005

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

## ORGANISATION OF THE JOŽEF STEFAN INSTITUTE

### **BOARD OF GOVERNORS**

### DIRECTOR

SCIENTIFIC COUNCIL

### RESEARCH DEPARTMENTS

### Physics

Theoretical Physics (F-1) Prof. Svjetlana Fajfer Low and Medium Energy Physics (F-2) 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<sup>1</sup>, Prof. Sašo Šturm<sup>2</sup>

> Synthesis of Materials (K-8) Prof. Darko Makovec

Advanced Materials (K-9) Prof. Danilo Suvorov<sup>1</sup>, Asst. Prof. Matjaž Spreitzer<sup>2</sup> 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. Gregor Dolanc Artificial Intelligence Laboratory (E-3) Prof. Dunja Mladenić Open Systems and Networks (E-5) Prof. Borka Jerman Blažič<sup>1</sup>, Asst. Prof. Tomaž Klobučar<sup>2</sup> Communication Systems (E-6) Prof. Mihael Mohorčič **Computer Systems Department (E-7)** 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

<sup>1</sup> until 31 March 2018 <sup>2</sup> since 1 April 2018

### CENTRES

Reactor Centre (RIC) Prof. Borut Smodiš Networking Infrastructure Centre (NIC) Dr. Jan Jona Javoršek Science Information Centre (SIC) Dr. Luka Šušteršič **Energy Efficiency Centre (EEC)** Stane Merše, M. Sc. **Centre for Knowledge Transfer in Information** Technologies (CT-3) Mitja Jermol, M. Sc. Milan Čopič Nuclear Training Centre (ICJT) 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 Smart Cities and Communities Centre (CSC & C) Matjaž Šteblaj, B. Sc. Center Factory of the Future (CFoF) Rudi Panjtar, B. Sc 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 For Experimental Particle Physicis 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. Purchase Department\* (U-3) Darko Korbar, M. Sc., MBA<sup>3</sup>, Regina Gruden, M. Sc.<sup>4</sup>, Dejan Ratković, B. Sc.<sup>4</sup> Finance and Accounting (U-4) Regina Gruden, M. Sc. Service for Business Informatics (U-5) Jože Kašman, B. Sc. International Project Office (U-6) Marja Mali, M. Sc.<sup>6</sup> Technical Services (TS) Aleš Cesar, B. Sc.

Support Units

Radiation Protection Unit (SVPIS) Matjaž Stepišnik, M. Sc. Quality Assurance (QA) Dr. Andrej Prošek Workshops Franc Setnikar, B. Sc.

### PARTICIPATION IN THE REGIONAL DEVELOPMENT OF RESEARCH

	Technolo	gy Centres
Ljubljana Technology Park Ltd.		
	Nanotesla Institute Ljubljana	Technology Centre for Production
University of Nova Gorica	Development Centre for Hydrogen	Automation, Robotics and Informatics
Jožef Stefan International	Technologies	(ARI)
Postgraduate School		
	Centres of Excellence	
Nanocenter - Center of Excellence in	Centre of Excellence NAMASTE	CEBIC Centre of Excellence for Biosensors
Nanoscience and Nanotechnology	Centre of Excenence NAMASTE	Instrumentation and Process Control
	Centre of Excellence for Polymer	CO NOT: Centre of Excellence for Low-
Centre of Excellence for Integrated Approaches in Chemistry and Biology	Materials and Technologies (PoliMaT)	Carbon Technologies
of Proteins (CIPKeBiP)	<b>EN-FIST Centre of Excellence</b>	Centre of Excellence for Space Sciences
		and Technologies SPACE-SI

\* Sales and Purchase Department (until 28 February 2018)

<sup>3</sup> until 28 February 2018 <sup>4</sup> 1 March-31 May 2018 <sup>5</sup> since 1 June 2018 <sup>6</sup> since 1 March 2018

## 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* Mr. Ivo Boscarol, *Pipistrel, d.o.o.* Prof. Sašo Džeroski, *JSI* Mrs. Martina Gašperlin, *Ministry for Economic Development and Technology* Prof. Primož Pelicon, *JSI* 

### SCIENTIFIC COUNCIL

Prof. Dragan Dragoljub Mihailovič, *President* Prof. Leon Cizelj Prof. Miran Čeh Prof. Svjetlana Fajfer Prof. Milena Horvat Prof. Đani Juričić, *Deputy President* Prof. Nada Lavrač Prof. Jadran Lenarčič Stojan Petrič, Kolektor, d. o. o., Idrija Prof. Jože Pungerčar, JSI Dr. Tomaž Savšek, TPV Group, d. o. o., Novo mesto Mrs. Kim Turk, Ministry of Education, Science and Sport Dr. Peter Vrtačnik, Ministry for Economic Development and Technology

Asst. Prof. Matej Lipoglavšek Prof. Barbara Malič Prof. Marko Mikuž Prof. Ingrid Milošev, *Deputy President* Prof. Gregor Papa Prof. Maja Remškar Prof. Boris Turk

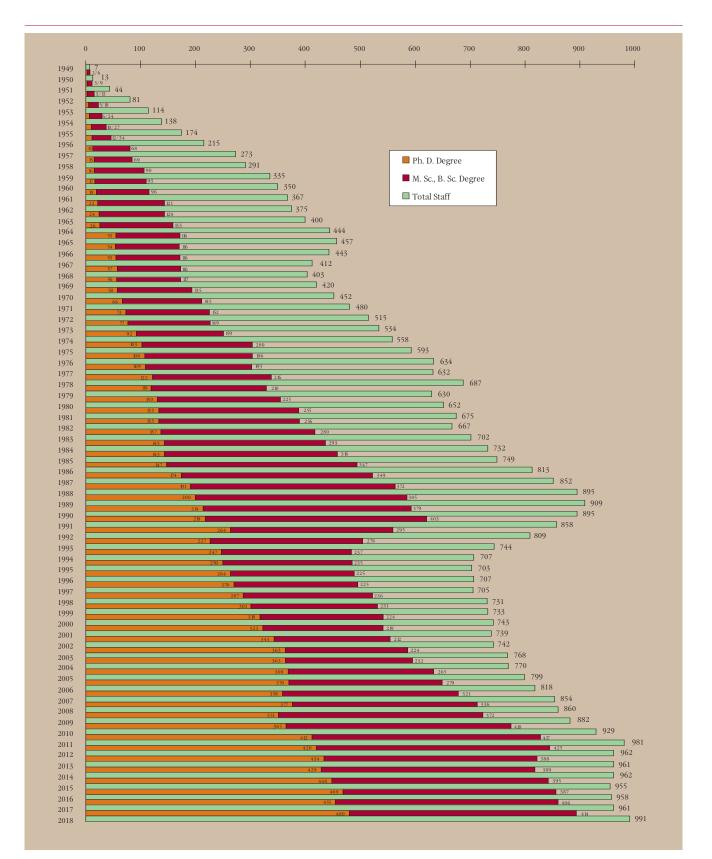
## INTERNATIONAL ADVISORY BOARD

- 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. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
  Prof. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
  Prof. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
  Prof. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
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  Prof. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
  Prof. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
  Prof. Karl A. Müller, Nobel Prize Winner, Universität Zürich, Zurich, Switzerland
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  Prof. Brian Clark, Auflus University, All Superson, Denmark
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- 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
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- Prof. Dietrich Munz, Universität Karlsruhe, Karlsruhe, Germany
- Prof. Günther Petzow, Max-Planck-Institut für Metallforschung, Stuttgart, Germany
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- 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

## 1949-2018



## 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)

Prof. Vito Turk, Director of the Jožef Stefan Institute from 1996 to 2005

## 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
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  Prof. Hans Fritz, Universität München, Munich, Germany
  Prof. Oskar Glemser<sup>‡</sup>, Universität Göttingen, Göttingen, Germany
  Prof. Paul Hagenmuller<sup>‡</sup>, Université de Bordeaux I, Bordeaux, France
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  Prof. Herbert W. Roesky, Universität Göttingen, Göttingen, Germany

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- 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<sup>⊕</sup>, Ludwig-Maximillians-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)	105
7. FP (COOPERATION: HEALTH, FOOD, AGRICULTURE/FISHERIES, BIOTECHNOLOGY, INFORMATION COMMUNICATION TECHNOLOGIES,	7
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	
ESI	30
OTHERS (COST, IAEA, JRC, ESA, NATO, CIP, CEF, EMPIR, LIFE+)	188
TOTAL	330

Bilateral cooperation	No. of projects	<b>Bilateral cooperation</b>
Austria	3	Japan
China	5	Macedonia
Germany	6	Montenegro
France	11	Russia
Croatia	7	Serbia
Hungary	2	Turkey
India	3	USA
		TOTAL

## INTERNATIONAL COOPERATION AGREEMENTS

### In 2018, international cooperation agreements were signed between the Jožef Stefan Institute and:

- 1. University of Rijeka (UNIRI), Rijeka, Croatia (U-1)
- 2. Ss. Cyril and Methodius University in Skopje, Skopje, The Former Yugoslav Republic of Macedonia (E-7, E-9)
- 3. Slovak Academy of Sciences, Bratislava, Slovakia (U-1)
- 4. Ikerlan S. Coop., Arrasate Mondragon (Gipuzkoa), Spain (CEU)
- 5. Nankai University (NKU), Tianjin, China (F-7)
- Brazilian Commission for Nuclear Energy, Nuclear Technology Development Center, CDTN/CNEN, Belo Horizonte, Minas Gerais, Brazil and Jožef Stefan International Postgraduate School, Ljubljana (O-2)

## COOPERATION WITH HIGHER-EDUCATION ESTABLISHMENTS

## FULL-TIME FACULTY MEMBERS

### Professors

- 1. Prof. Denis Arčon, University of Ljubljana, Faculty of Mathematics and Physics
- 2. Prof. Iztok Arčon, University of Nova Gorica
- 3. Asst. Prof. Rok Bojanc, University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies
- 4. Prof. Janez Bonča, University of Ljubljana, Faculty of Mathematics and Physics
- 5. Asst. Prof. Marko Bračko, University of Maribor, Faculty of Chemistry and Chemical Engineering
- 6. Prof. Dean Cvetko, University of Ljubljana, Faculty of Mathematics and Physics
- 7. Prof. Mojca Čepič, University of Ljubljana, Faculty of Education
- 8. Prof. Martin Čopič, University of Ljubljana, Faculty of Mathematics and Physics
- 9. Prof. Janez Dolinšek, University of Ljubljana, Faculty of Mathematics and Physics
- 10. **Prof. Irena Drevenšek Olenik**, University of Ljubljana, Faculty of Mathematics and Physics
- 11. Prof. Svjetlana Fajfer, University of Ljubljana, Faculty of Mathematics and Physics
- 12. Asst. Prof. Darja Fišer, University of Ljubljana, Faculty of Arts
- 13. Prof. Boštjan Golob, University of Ljubljana, Faculty of Mathematics and Physics
- 14. Prof. Tomaž Gyergyek, University of Ljubljana, Faculty of Electrical Engineering
- 15. Asst. Prof. Branko Kavšek, University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies
- 16. **Prof. Samo Korpar**, University of Maribor, Faculty of Chemistry and Chemical Engineering
- 17. Prof. Janko Kos, University of Ljubljana, Faculty of Pharmacy
- 18. Prof. Samo Kralj, University of Maribor, Faculty of Education
- 19. Prof. Peter Križan, University of Ljubljana, Faculty of Mathematics and Physics
- 20. **Prof. Brigita Lenarčič**, University of Ljubljana, Faculty of Chemistry and Chemical Technology
- 21. Prof. Marko Mikuž, University of Ljubljana, Faculty of Mathematics and Physics
- 22. Prof. Igor Muševič, University of Ljubljana, Faculty of Mathematics and Physics
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January 17, 2018: Masaki Saito Tokyo Institute of Technology, Tokyo, Japan *Protected Plutonium Production by Transmutation of Minor Actinides* 

January 31, 2018: Denis Arčon Jožef Stefan Institute and Faculty of Mathematics and Physics, University of Ljubljana *Frustration in Antiferromagnetic Systems – A Laboratory for New States of Matter* 

February 7, 2018: Stéphane P. A. Bordas University of Luxembourg, Luxembourg, Cardiff University, Cardiff, United Kingdom *Predicting Failure in Aircraft Structures – Simulating Fracture across Scales and Times* 

February 14, 2018: Miha Krofel Biotechnical Faculty, University of Ljubljana, Ljubljana *Role of Science in Management of Large Beasts* 

March 19, 2018: Philippe Marcus CNRS - Chimie ParisTech - PSL University, France *Metal Surfaces and Thin Oxide Films: From Nanostructures to Corrosion Protection* 

March 20, 2018: Dragan Živadinov Avgust Černigoj and Teater-Masse

March 21, 2018: Duncan Haldane Princeton University, USA *Entanglement: Einstein's Gift to Quantum Mechanics* 

March 21, 2018: Oussama Khatib Stanford University, USA Ocean One - A Robotic Avatar for Deep-Sea Exploration

March 22, 2018: **Slobodan Žumer** Jožef Stefan Institute and University of Ljubljana *Frustrated Liquid-Crystalline Ordering as a Key to Topological Soft Matter* 

March 23, 2018: Tony Veale University College Dublin, Ireland *What will it Take to Give Machines a Real Sense of Humour* 

May 8, 2018: Nicolae Victor Zamfir Extreme Light Infrastructure – Nuclear Physics, Bucharest, Romania High-Intensity Laser Infrastructure Center for Nuclear Physics Research May 9, 2018: Edouard Hannezo Institute of Science and Technology Austria, Vienna, Austria *A Quantitative Self-Organized Model of Branching Morphogenesis* 

May 16, 2018: Kenji Uchino The Pennsylvania State University, State College, USA *Piezoelectric Energy Harvesting Systems* 

May 30, 2018: Roman Jerala National Institute of Chemistry, Ljubljana, Slovenia Design of Molecular Origami for New Molecular Machines and for Control of Cell Function

June 1, 2018: **Ivan I. Smalyukh** University of Colorado, Boulder, USA *A Journey with Bacteria: From Waste to Nematic Colloids and Gels and to Smart Windows* 

June 27 2018: **Robert Jeraj** University of Wisconsin, Madison, USA, University of Ljubljana *Role of Medical Physics in the Era of Precision Medicine* 

November 7, 2018: Ute Resch-Genger Federal Institute for Materials Research and Testing, Berlin, Germany Biophotonics and Analytics - Photoluminescence Properties of Nanocrystals and Surface Group Analysis

November 22, 2018: **Rafal E. Dunin-Borkowski** Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany *Electromagnetic Field Mapping at the Nanoscale in the Transmission Electron Microscope* 

December 6, 2018: **Qi-Huo Wei** Advanced Materials and Liquid Crystal Institute in Department of Physics, Kent State University, Kent, USA *Orient Molecules as You Wish* 

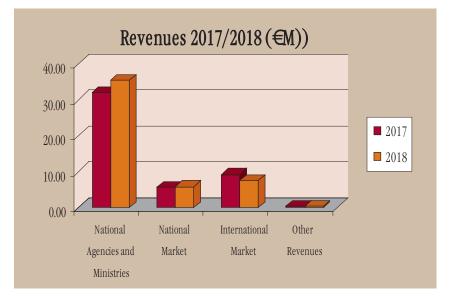
December 12, 2018: **Peter Jeglič** Jožef Stefan Institute **Quantum Technologies with Cold Atoms** 

December 19, 2018: **Stephane Mangin** Institut Jean Lamour, UMR CNRS 7198 - Universite de Lorraine, Nancy, France *Engineering Materials for All Optical Magnetic Recording* 

## FINANCING

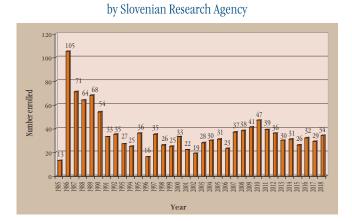
## REVENUES JSI (€) AND NUMBER OF PROJECTS

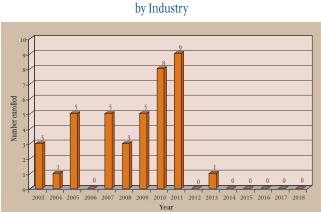
		Contribution		Contribution		No. of Projects
	2018	2018	2017	2017	Index 2018/2017	in 2018
National Agencies and Ministries	35,471,296	72.4 %	32,265,588	67.9 %	109.9	371
National Market	5,820,996	11.9 %	5,725,866	12.0 %	101.7	393
International Market	7,533,096	15.4 %	9,183,505	19.3 %	82.0	312
Other Revenues	161,911	0.3 %	359,533	0.8 %	45.	
TOTAL	48,987,299	100.0 %	47,534,492	100.0 %	103.1	1076



## POSTGRADUATES FINANCED

## 1985-2018





### Annual Report 2018

# JSI UNDERGRADUATE SCHOLARSHIPS

1977-2018

Year		FMF	FKKT	FKKT	NTF	FDV	FA	BF	FE and	Other	FG and	UNG	IPS	Total
			UNI LJ	UNI MB					FRI	UNI LJ	FERI			
1983	125	39	105						59	12	1			341
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
2017	11	2	4					2	7				12	38
2018	9	3	5					2	6	1	1		7	34
TOTAL	457	111	443	25	13	8	4	67	492	34	21	11	67	1753
FMF FKKT (Uni-Lj) FKKT (Uni-Mb) NTF FDV FA BF							ity of Maribor							

Economics, Faculty of Medicine, University of Ljubljana

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## PATENTS GRANTED

- Sergey Grigorievich Psakhie, Izraillevich Marat Lerner, Elena Alekseevna Glazkova, Olga Vladimirovna Bakina, Olga Vasiljeva, Georgy Mikhaylov, Boris Turk, Low-dimensional structures of organic and/or inorganic substances and use thereof, US10105318 (B2), US Patent and Trademark Office, 23. 10. 2018.
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- Norbert Schaschke, Olga Vasiljeva, Georgy Mikhaylov, Boris Turk, Cathepsinbinding compound bound to a liposome and its diagnostic and therapeutic use, EP2723387 (B1), European Patent Office, 18. 04. 2018.
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- Xinzheng 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, EP2977815 (B1), European Patent Office, 05. 09. 2018.

- Irena Ramšak, Marija Razpotnik, Katja Makovšek, Danjela Kuščer, Silvo Drnovšek, Janez Holc, Production method of steatite ceramics with improved electrical properties, EP3230232 (B1), European Patent Office, 15. 08. 2018.
- Irena Ramšak, Marija Razpotnik, Janez Holc, Danjela Kuščer, Method for producing non-alkaline steatite ceramics with improved electrical properties, EP3233755 (B1), European Patent Office, 10. 10. 2018.
- Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, Functionalized hydroxyapatite/gold composites as "green" materials with antibacterial activity and the process for preparing and use thereof, EP2863751 (B1), European Patent Office, 25. 07. 2018.
- Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, A method to produce foam glasses, EP2966044 (B1), European Patent Office, 26. 09. 2018.
- Ana Mladenovič, Primož Oprčkal, Nina Kržišnik, Radmila Milačič, Janez Ščančar, Andrijana Sever Škapin, Process for obtaining health - and environment acceptable construction materials from the soil containing water soluble compounds of heavy metals, EP3131688 (B1), European Patent Office, 24. 01. 2018.
- Ana Mladenovič, Primož Oprčkal, Radmila Milačič, Janez Ščančar, Janja Vidmar, Andrijana Sever Škapin, Peter Nadrah, Alenka Mauko Pranjić, Mirko Šprinzer, Method and system for the potabilization of effluents from biological WWTPS, SI25327 (A), Urad RS za intelektualno lastnino, 29. 06. 2018.
- Matej Holc, Ita Junkar, Gregor Primc, Miran Mozetič, Jernej Iskra, Primož Titan, Method of treating garlic cloves, SI25440 (A), Urad RS za intelektualno lastnino, 31. 12. 2018.

## ART EXHIBITIONS AT THE JSI

Polona Lovšin, 15 January-22 February Jernej Forbici, 26 February-15 March Avgust Černigoj, 19 March-19 April Marija Flegar, 23 April-10 May Mirsad Begić, 14 May-7 June Tajda Lekše, 11 June-22 June Miro Starič, 26 June-18 July Alenka Štante, 23 July-5 September Mateja Kavčič, 10 September-11 October Andrej Pavlič, 15 October-7 November Eva Lucija Kozak, 12 November-5 December Marjana Pahor, 10 December-9 January 2019



Mirsad Begić at the opening of his exhibition

## **REVIEW OF PUBLICATIONS**

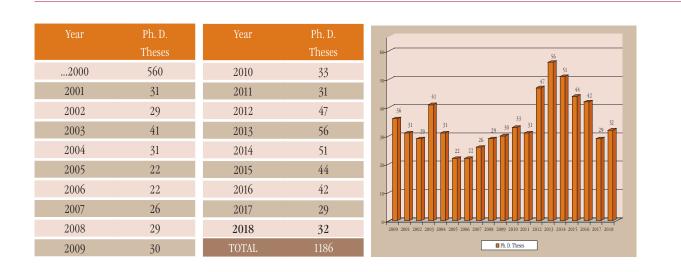
### FOR 2018

Department	Original Articles*	Books	Patent Appl. and	Ph. D. Theses
Department	Original Articles*	DOOKS	Grants	Pfl. D. Theses
Department of Theoretical Physics (F-1)	84	2		
Department of Low and Medium Energy Physics (F-2)	73	1		3
Department of Thin Films and Surfaces (F-3)	9			
Department of Surface Engineering and Optoelectronics (F-4)	70		2	1
Department of Solid State Physics (F-5)	118	5	2	4
Department for Complex Matter (F-7)	41		1	
Department of Reactor Physics (F-8)	106	2		2
Department of Experimental Particle Physics (F-9)	128	1		3
Department of Inorganic Chemistry and Technology (K-1)	18			
Department of Physical and Organic Chemistry (K-3)	22			1
Electronic Ceramics Department (K-5)	53		3	1
Department for Nanostructured Materials (K-7)	55			3
Department for Synthesis of Materials (K-8)	15			
Department for Advanced Materials (K-9)	42		2	1
Department of Biochemistry, Molecular and Structural Biology (B-1)	15		2	3
Department of Molecular and Biomedical sciences (B-2)	17			
Department of Biotechnology (B-3)	34			2
Department of Environmental Sciences (0-2)	93		3	2
Department of Automation, Biocybernetics and Robotics (E-1)	47		1	1
Department of Systems and Control (E-2)	23			
Artificial Intelligence Laboratory (E-3)	49	3		2
Laboratory for Open Systems and Networks (E-5)	11	1		
Department of Communication Systems (E-6)	47	2	1	
Computer Systems Department (E-7)	29	1		1
Department of Knowledge Technologies (E-8)	114			2
Department of Intelligent Systems (E-9)	72			1
Department of Reactor Engineering (R-4)	58	1		1
Reactor Infrastructure Centre (RIC)	14			
Energy Efficiency Centre (EEC)	11			
Centre for Electron Microscopy and Microanalysis (CEMM)	13			
Centre for Knowledge Transfer in Information Technologies (CT-3)	1			
Radiation Protection Unit (SVPIS)	1	1		
Centre for Technology Transfer and Innovation (CTT)	3			
Center for Smart Cities and Communities (CSC&C)	11			
Center Factory of the Future (CFoF)	1		1	
Jožef Stefan Institute	1338	17	16	32

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

## **COMPLETED THESES**

### UNTIL 2018



## AWARDS AND APPOINTMENTS

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

### Zois Certificate of Recognition

#### Saša Prelovšek Komelj

Presented with the Zois Certificate of Recognition for important achievements in theoretical particle physics

### Tadej Rojac

Presented with the Zois Certificate of Recognition for significant achievements in researching the synthesis and characterization of high-temperature piezoelectric ceramics based on bismuth ferrite

### JSI AWARDS AND APPOINTMENTS

### The Jožef Stefan Golden Emblem Prize

presented to the following for doctoral theses with high impact :

#### Dr. Boris Brus

Structure-based design and evaluation of potential immunomodulatory and neuroprotective agents

### Dr. Tina Lebar

Design of genetic regulatory networks based on DNA binding proteins

Dr. Zala Lenarčič Nonequilibrium properties of Mott insulators

### JSI Director's fund

Tadej Petrič and Dragi Kocev

for the project entitled "CoBoTaT – Laboratory for Advancing Collaborative Robot Behaviors in Physical Human-Robot Interaction Scenarios"

## OTHER SELECTED AWARDS TO JSI RESEARCHERS

**Department for Nanostructured Materials**, The European project REProMag, German Prize for Efficient Use of Raw Materials 2017 (Deutscher Rohstoffeffizienz-Preis 2017, awarded in January 2018

Aleš Berlec, Lapanje plaque, Ljubljana. Awarded by the Slovenian Biochemical Society for expert and organizational work in society.



The winners of the Jožef Stefan Golden Emblem Prize: Dr. Tina Lebar and Dr. Zala Lenarčič with Dr. Miro Cerar, Prime Minister and Prof. Jadran Lenarčič, Director of JSI

Jani Bizjak, Anton Gradišek, Matjaž Gams, Award for the best innovation for public research organization, Ljubljana, The 11th International Technology Transfer Conference, The ultimate European assistant for the elderly

Jani Bizjak, Matjaž Gams, Anton Gradišek, Best innovation from public research organizations, TEE-The ultimate European assistant for the elderly, at IS 2018

Jani Bizjak, Vid Drobnič, Matjaž Gams, Martin Gjoreski, Vito Janko, Mitja Luštrek, Matej Marinko, Miha Mlakar, Nina Reščič, Gašper Slapničar, SHL Challange – Sussex-Huawei Locomotion and Transportation Recognition Challenge, 1<sup>st</sup> Place Award; Singapore; Dr. Hristijan Gjoreski, University of Sussex (UK) & Ss. Cyril and Methodius University (MK), Dr. Lin Wang, University of Sussex (UK), Dr. Daniel Roggen, University of Sussex (UK), Dr. Kazuya Murao, Ritsumeikan University (JP), Dr. Tsuyoshi Okita, Kyushu Institute of Technology (JP); method for the recognition of locomotion activity from smartphone sensors

Marko Bračko, Recognition award from the University of Maribor for a scientific research project, art and educational work for higher professors, science teachers and other college associates for special successes, achievements and credits, Maribor, Faculty of Chemistry and Chemical Engineering.

Miha Dežman, Best overall conference contribution for the ICT study programme, Piran, Slovenia, IPSS conference expert commission - 10th International Postgraduate School Students Conference, Elbow assistance exoskeleton to facilitate high-level control design. Vid Drobnič, Matjaž Gams, Martin Gjoreski, Vito Janko, Mitja Luštrek, Matej Marinko, Nina Reščič, Gašper Slapničar, SHL Challange – Sussex-Huawei Locomotion and Transportation Recognition Challenge, 2<sup>nd</sup> Place Award; Singapore; Dr. Hristijan Gjoreski, University of Sussex (UK) & Ss. Cyril and Methodius University (MK), Dr. Lin Wang, University of Sussex (UK), Dr. Daniel Roggen, University of Sussex (UK), Dr. Kazuya Murao, Ritsumeikan University (JP), Dr. Tsuyoshi Okita, Kyushu Institute of Technology (JP); method for recognition of locomotion activity from smartphone sensors

Damir Hamulić, Ingrid Milošev, Peter Rodič, Dolores Zimerl, Award for best invention/innovation with the commercial potential at 11. ITTC in 2018.

James Alexander Hodson, Best paper on long-term investments - Trading on Talent: Human Capital and Firm Performance, Northern Finance Association 2018 (NFA 2018), 21–23 Sept. 2018 Charlevoix, Canada

Tadej Holler, Romain Grosseuvres, Alexandre Bleyer, Ludovic Maas, Mantas Povilaitis, "ETSON Award 2018" for collaborative paper of junior experts (ETSON Award, Brussels, Belgium), European Technical Safety Organisations Network, for the paper "Temperature conditions effect on hydrogen-air flame propagation in the ENACCEF2 experimental facility"

Tadej Holler, Ed M.J. Komen, Ivo Kljenak, Young author award (NENE 2018 conference, Portorož, Slovenia), Nuclear Society of Slovenia, for the paper "Weighted laminar flame speed approach to simulating large-scale hydrogen deflagration experiment"

Borka Jerman Blažič, Recognition from The Program Committee of the Multiconference Information Society 2018 for the life work: "The First Lady of the Slovenian Internet", Ljubljana, October 12, 2018

Borka Jerman Blažič, Recognition award, "Hack Istanbul 2018" conference, Istanbul, Turkey, September 21 – 23, 2018.



The winners of Zois Certificates of Recognition: Prof. Saša Prelovšek Komelj and Asst. Prof. Tadej Rojac

Sonja Jovanović, Best oral presentation of the 20<sup>th</sup> Conference YUCOMAT 2018, Herceg Novi, Montenegro: "Synthesis of antimicrobial cobalt ferrite/gold nanocomposites".

Matej Kocen, Award for the best poster and oral presentation at the 26<sup>th</sup> International Conference on Materials and Technology, 26 ICM&T, Portorož, Slovenia, 3–5 October 2018. Title of the awarded contribution: "Capturing the Sun in a tungsten 'box'" (coauthors: Petra Jenuš, Saša Novak Krmpotič, Andreja Šestan)

Janez Kokalj, Matjaž Leskovar, Mitja Uršič, Best poster award (NENE2018 conference, Portorož, Slovenia), Nuclear Society of Slovenia, for the paper "Model for premixed layer formation in stratified melt-coolant configuration"

Aleš Lapanje, OECD Innovation Award: Biocatalytic Aggregates for the Conversion of Biomass Invasive Plants into Useful Products. Paris, 19-20 November, 2018

Jasmina Masten, Prešeren's Award for a Master's thesis, entitled: Parameters of quality of salads, tomatoes and peppers from shops

Ingrid Milošev, Peter Rodič, Krka Prize for secondary-school research papers - award for mentorship.

Ingrid Milošev, Peter Rodič, Silver Award at the 52<sup>th</sup> Meeting of young researchers Slovenia - award for mentorship.

Mimoza Naseska, Best poster award, International Workshop Quantum Complex Matter (QCM 2018) and Frontiers Condensed Matter Physics (FCMP), 11–15 June 2018, Rome, Italy, poster "Optical quench and recovery of SDW state SeFe<sub>2</sub>As<sub>2</sub> and EuFe<sub>2</sub>As<sub>2</sub>"

Mimoza Naseska, Best poster award, 2018 Low Energy Electrodynamics of Solids (LEES) conference, 24–29 June 2018, Portonovo, Italy, poster "Optical quench and recovery of SDW state SeFe,As, and EuFe,As,"

Mimoza Naseska, Faculty Prešeren Award for her work titled "Ultrafast Spin Density Wave dynamics at intense optical pulse excitation", supervisor Asst. Prof. Tomaž Mertelj

Nives Ogrinc, Vrzel, J., Ludwig, R., Award for the best presentation at the conference: Understanding of groundwater and surface water as a single system in the Ljubljansko polje, Slovenia. GLOBAQUA final conference: water river management under water scarcity and multiple stressors, 17–19 December 2018, Barcelona, Spain.

Nives Ogrinc, Tea Zuliani, Staša Hamzić Gregorčič, Best Poster Award: Award ISO-FOOD: Optimisation of the method for Sr isolation from the matrix for reliable determination of 87Sr/86Sr isotope ratio by MC-ICP-MS in milk. 10<sup>th</sup> Jožef Stefan International Postgraduate School Students' Conference and 12<sup>th</sup> Young Researchers' Day, 10–11 May 2018, Piran, Slovenia. Ljubljana.

Nives Ogrinc, Plestenjak, Gregor, Vodnik, Dominik, Krajnc, Bor, Ferlan, Mitja, Mihelič, Rok, Eler, Klemen, Award for poster: Could the additional air supply enhance the decomposition processes in sludge drying reeds beds? 16<sup>th</sup> IWA International Conference on Wetland Systems for Water Pollution Control, 30 September - 4 October 2018, Valencia, Spain. Valencia: International Water Association. **Tadej Petrič, Leon Žlajpah**, Best regular paper award, The 27<sup>th</sup> International Conference on robotics in Alpe-Adria-Danube Region, Virtual Guides for Redundant Robots Using Admittance Control for Path Tracking Tasks, Patras, Greece.



The winners of the JSI Director's fund award: Asst. Prof. Tadej Petrič and Dr. Dragi Kocev

**Rudolf Podgornik**, Publons Peer Review Award for the year 2018 for reviewing manuscripts submitted to scientific journals. His reviewing work was also recognized by the American Chemical Society (Washington, DC, USA) as Marsha I. Lester, the editor of The Journal of Chemical Physics (Melville, NY, USA), mentioned him as one of the best reviewers of the journal.

**Benjamin Podmiljšak**, Award for the best poster at the 2<sup>nd</sup> IEEE Conference on Advances in Magnetics; AIM2018, La Thuile, Italy, 3–10 February 2018. Title of the awarded contribution: "Tailored metal injection moulding of isotropic NdFeB hard magnets based on recycled powders with and without Nd additions".

Saša Prelovšek Komelj, Excellent in science 2018 awarded by Slovenian Research Agency ARRS for most important achievements (10 achievements in a given year are chosen for natural sciences) awarded achievement: Pion-nucleon scattering in the Roper channel from lattice QCD, Physical Review D 95 (2017) 014510, C.B. Lang, L. Leskovec, M. Padmanath in S. Prelovšek

Tadej Rojac, Young investigator award for his pioneering work in processing of chemically complex ferroelectric ceramics, IEEE Ultrasonics Ferroelectrics and Frequency Control Society

Urša Tiringer, Gavrilo Šekularac, Young Author's EFC Poster Prize EUROCORR 2018

Aneta Trajanov, Best Poster Presentation Award, 19th Open Conference of the IFIP WG 8.3. on Decision Support Systems, 13–15 June 2018, Ljubljana, Slovenia.

Marija Vukomanović, Danilo Suvorov, Srečo Davor Škapin, Silver medal for the invention of "Functionalized hydroxyapatite/gold composites as "green" materials with antibacterial activity and the process for preparing and use thereof", 16<sup>th</sup> International Exhibition of Innovations (ARCA 2018), Zagreb, Croatia.

**Primož Ziherl**, Advisor of the Year award for 2018 awarded by the Young Academy (Ljubljana).

## **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**

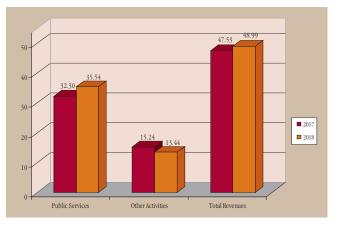
- 1. Aerosol, d.o.o., Ljubljana
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- 5. Bioiks, d.o.o., Ljubljana
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- 21. GKN Driveline Slovenija, d.o.o., Zreče
- 22. The Chamber of Commerce and Industry of Slovenia, Ljubljana
- 23. Ljubljana Exhibition and Convention Centre, Ljubljana
- 24. Hidria Holding, d.o.o., Ljubljana
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- 36. Kekon, d.o.o., Žužemberk
- 37. National Institute of Chemistry, Ljubljana
- 38. KMZ Zalar Miran, s.p., Ljubljana
- 39. Knauf Insulation, d.o.o., Škofja Loka
- 40. Kolektor Group, d.o.o., Idrija
- 41. Kolektor Sikom, d.o.o., Idrija
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- 44. Lek, d.d., Ljubljana
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- 47. Mahle Electric Drives Slovenija, d.o.o., Šempeter pri Gorici
- 48. Marjetica, d.o.o., Koper
- 49. Ministry of Economic Development and Technology Metrology Institute of the Republic of Slovenia, Ljubljana, Celje

- 50. Ministry of Economic Development and Technology, Ljubljana
- 51. Ministry of Infrastructure, Ljubljana
- 52. Ministry of Education, Science and Sport, Ljubljana
- 53. Ministry of Agriculture, Forestry and Food, Administration of the Republic of Slovenia for Food Safety, Veterinary Sector and Plant Protection, Ljuljana
- 54. Ministry of the Interior, Ljuljana
- 55. Ministry of Defence, Ljuljana
- 56. Ministry of the Environment and Spatial Planning, Ljuljana
- 57. Ministry of the Environment and Spatial Planning, Slovenian Environment Agency, Ljuljana
- 58. Ministry of the Environment and Spatial Planning, Slovenian Nuclear Safety Administration, Ljubljana
- 59. Ministry of Health, Slovenian Radiation Protection Administration, Ljubljana
- 60. Ministry of Health, Chemicals Office of the Republic of Slovenia, Ljubljana
- 61. National institute of Public Health, Ljubljana
- 62. NELA razvojni center, d.o.o., Železniki
- 63. Krško Nuclear Power Plant, d.o.o., Krško
- 64. Institute of Oncology, Ljubljana
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- 70. Reodom, d.o.o., Grosuplje
- 71. RLS Merilna tehnika, d.o.o., Komenda
- 72. RŽV, d.o.o., Gorenja vas
- 73. SiEVA, d.o.o., Šempeter pri Gorici
- 74. SIJ ZIP center, d.o.o., Ravne na Koroškem
- 75. Government Office for Development and European Cohesion Policy, Ljubljana
- 76. Splošna bolnišnica "Dr. Franca Derganca", Šempeter pri Gorici
- 77. Splošna bolnišnica, Novo mesto
- 78. Syntech, d.o.o., Ljubljana
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- 84. University of Ljubljana, Faculty of Natural Sciences and Engineering, Ljubljana
- 85. University of Ljubljana, Faculty of Mechanical Engineering, Ljubljana
- 86. University of Maribor, Maribor
- 87. University of Maribor, Faculty of Mechanical Engineering, Maribor
- 88. University Rehabilitation Institute, Republic of Slovenia Soča, Ljubljana
- 89. Vacutech, d.o.o., Ljubljana
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- 91. Zavod Tehnološka mreža ICT, Ljubljana
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- 93. Institute of Occupational Safety, Ljubljana
- 94. Žito, d.o.o., Ljubljana

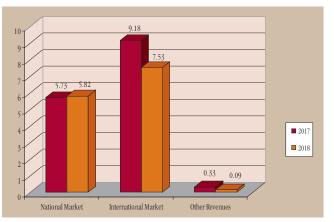
## INSTITUTE IN NUMBERS

### 2017-2018

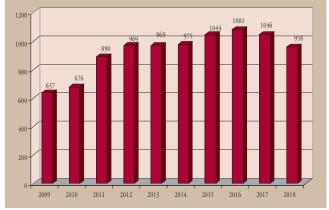
COMPARISON OF REVENUES (€M)



### REVENUES FROM OTHER ACTIVITIES (€M)

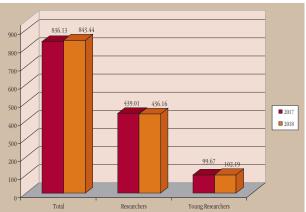


### NUMBER OF PUBLICATIONS IN THE WEB OF SCIENCE\*

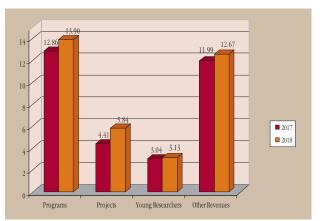


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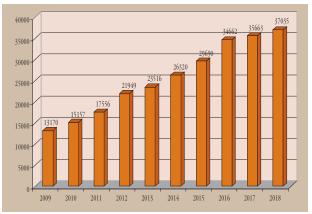
EMPLOYEES (FTE)



### REVENUES FROM PUBLIC SERVICES (€M)



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## **RESEARCH DEPARTMENTS**

## DEPARTMENT OF THEORETICAL PHYSICS F-1

In 2018, members of the program group THEORY OF NUCLEUS, ELEMENTARY PARTICLES AND FIELDS continued with reserach in the areas of hadronic physics, quantum chromodynamics, effective field theory of electroweak decays of mrsons, unified theory and precise calculations in the three-body systems.

We determined the energies and spin-parities of the low-lying and excited charmonia within lattice QCD. Charmonia with various momenta and all spins  $J \le 3$  were considered, neglecting the strong decays of resonances. We performed the first lattice QCD simulation of the proton-I/  $\psi$  scattering in the channels and the energy range, where LHCb discovered exotic pentquarks  $Pc'uudcc^{-}$  in 2015. Our lattice results indicate that the coupling of the proton- $I/\psi$  channel with the other two-hadron channels might be responsible for Pc resonances in experiments.

We investigated the effects of new physics in B semi-leptonic decays and K decays to pi and two neutrinos. First we considered the impact of leptoquarks, which might explain either RK(\*) or RD(\*) anomalies on K -> pi nu bar nu decays. We found that contributions of leptoquark-driven new physics might reduce the observed branching Head: ratio up to 20%. Hypothetical spin-2 particles might contribute to B-> K(\*) mu + mu- decay due to the dimension Prof. Svjetlana Fajfer 8 effective operators and can be observed only in forward-backward asymmetries. We succeeded in constructing a grand unified model containing the weak triplet and doublet of leptoquarks explaining B meson anomalies and

not being in a conflict with any flavour physics low-energy observables, as well as any LHC results.

We introduced a set of clockwork models of flavour that can naturally explain the large hierarchies of the Standard Model quark masses and mixing angles. We investigated the bounds on light pseudoscalars that arise from a variety of collider searches. We proposed a direct measurement of the CKM element V\_{td} at the LHC.

In the context of left-right symmetry, we revisited the Keung-Senjanović production of right-handed  $W_{R}$  bosons and heavy neutrinos N at highenergy colliders. We developed a multibinned analysis to estimate the sensitivity for the range of N masses from the standard and merged prompt to displaced vertices and the invisible N region. The sensitivity of the LHC with 300/fb luminosity ranges from 5 to beyond 7 TeV, while the future 33(100) TeV reach with 3/ab extends to 12(26) TeV.

By adding a 54-dimensional representation in the SO(10) unified theory with bosonic supersymmertric partners above 100 TeV we described the Yukawa sector with only two symmetric matrices. We showed some explicit examples of non-perturbative supersymmetric asymptotically safe theories in accord with the a-theorem, among others SQCD with two adjoints and some theories with a large number of flavours.

### Some outstanding publications in the past three years

- Haisch, Ulrich, Kamenik, Jernej, Malinauskas, Augustinas, 1 Spira, Michael. Collider constraints on light pseudoscalars. The journal of high energy physics, ISSN 1029-8479, 2018, vol. 2018, št. 3, str. 178-1-178-19, doi: 10.1007/JHEP03(2018)178. [COBISS. SI-ID 31412519]
- 2. Babu, K. S., Bajc, Borut, Saad, Shaikh. Resurrecting minimal Yukawa sector of SUSY SO(10). The journal of high energy physics, ISSN 1029-8479, 2018, vol. 2018, no. 10, str. 135-1-135-24, doi: 10.1007/JHEP10(2018)135. [COBISS.SI-ID 32040487]

Our lattice QCD results indicate that the exotic charmed pentaquark resonances in experiments might arise due to the coupling of the proton- $I/\psi$ channel with the other two-hadron channels.

We proposed the minimal supersymmetric SO(10) unified theory and found some examples of supersymmetric asymptotic safety.

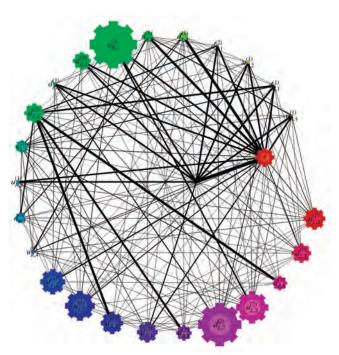


Figure 1: Schematic representation of the spectrum and decay patterns of fermionic states in an example model of clockwork flavour for quarks.



## The group of SOLID STATE THEORY AND STATISTICAL PHYSICS has been investigating the equilibrium and non-equilibrium properties of materials with strongly correlated electrons, nanosystems, as well as the properties of complex networks.

We continued the research of disordered quantum models, which exhibit the phenomenon of many-body localization and a non-ergodic behaviour of physical quantities. In relation to experiments on cold atoms the most relevant model is the disordered Hubbard chain, where we confirmed the absence of full localization via the local integrals of motion. With the derivation of an effective squeezed spin model we explained the sub-diffusive spin dynamics, being the consequence of a singular distribution of exchange couplings. Similar sub-diffusive dynamics has been found for a particle moving in a disordered chain and coupled to hard-core bosons.

In relation with local experiment we continued the investigation of frustrated spin models, which are candidates for the existence of spin-liquid phases. By calculating numerically, the temperature dependence of several physical guartities are confirmed the possibility of such a regime.

With the use of numerical simulations we described measurements of a cold atom experiment and by calculating the charge susceptibility and the diffusion constant explained the behavior of resistivity in bad metals at high temperature. quantities, we confirmed the possibility of such a regime.

We consider the propagation of a quantum particle in a random chain, assisted by the coupling to dispersive bosons. Time evolution treated with rate equations for hopping between localized states reveals a qualitative difference between the dynamics due to non-interacting bosons and hard-core bosons. In the first case the transient dynamics is sub-diffusive, but multi-boson processes allow for long-time normal diffusion, while hard-core effects suppress multi-boson processes leading to persistent numerical results for a full many body evolution.

sub-diffusive transport, consistent with numerical results for a full many-body evolution.

By using the Finite-Temperature Lanczos Method (FTLM) we studied the behaviour of charge susceptibility, diffusion and resistivity in a model of strongly correlated electrons and successfully described the cold atom experiment. We realized that the charge susceptibility shows strong temperature dependence down to surprisingly low temperatures and that it is responsible for the resistivity being larger than the Mott-Ioffe-Regel limit.

We explored phenomena in complex hybrid semiconductor-superconductor devices, such as a double quantum dot in InAs quantum wire. We explored the case where one of the leads is superconducting and the other is normalstate, as well as the case of two superconducting leads. In the first case we determined the phase diagram of ground states delineated by the crossing of Yu-Shuba-Rusinov states across the Fermi level. In the second case we studied the Josephson current through the device and we have showed that it is possible to distinguish the singlet state of two antiferromagnetically coupled spins from the singlet state of two separate Kondo clouds.

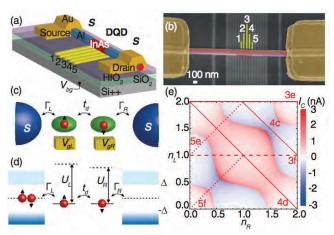


Figure 2: Hybrid quantum device for measuring the Josephson current across trapped electrons, model system and computed critical current.

We investigated the impact of topological constraints on the collective dynamics in driven physical, biological and social systems. The underlying structures represented by networks are suitably parameterized by simplexes (triangles, tetrahedrons, etc.) that merge into larger complexes and possess an emergent hyperbolic geometry. In the particular system, the exact structure embodies the processes of self-assembly of preformatted nanoparticle groups, or details of the brain-to-brain coordination recorded by EEG signals and self-organized dynamics in social knowledge-creation processes. In the compact 2-dimensional geometry of ferromagnetic films, the actual sample shape affects the motion of the extended domain wall and changes the hysteresis-loop criticality.

We studied the entanglement entropy in eigenstates of the paradigmatic model of quantum phase transitions, i.e., the one-dimensional Ising model in a transverse magnetic field. We showed that the average entanglement entropy (over all eigenstates) carries information about the critical value of the magnetic field.

We investigated the influence of the spin-orbit coupling in correlated transition-metal oxides. We investigated under which circumstances the

spin-orbit coupling importantly influences the electronic correlations. We also investigated the influence of electronic correlations on spectroscopical manifestations of the influence of the spin-orbit coupling, such as the liftings of the degeneracies.

A promising method of qubit manipulation in quantum information processing applications is the manipulation where the Rashba effect in non-adiabatic systems induces quantum phases, including the spin rotation. By the virtue of exact unitary transformations we analysed stability properties of qubit transformations and the corresponding fidelity as influenced by the Ornstein-Uhlenbeck coloured noise of driving fields and coupled to thermal baths.

We studied the electron transport in the Bernevig-Hughes-Zhang model undergoing a slow quench between different topological regimes. We showed that the deviations from the ground-state spin Hall conductivity as a function of the quench time follow the Kibble-Zurek scaling. We improved the Luttinger field approach to calculating the time-dependent currents through a nanoscopic device as a result of switching on a temperature gradient across the device. Using density functional theory and kinetic Monte Carlo simulations we studied the morphology evolution of different surface orientations of the magnesium crystal.

### Some outstanding publications in the past three years

- Peter T. Brown, Debayan Mitra, Elmer Guardado-Sanchez, Reza Nourafkan, Alexis Reymbaut, Charles-David Hébert, Simon Bergeron, A.-M. S. Tremblay, Jure Kokalj, David A. Huse, Peter Schauss, Waseem S. Bakr, *Bad metallic transport in a cold atom Fermi-Hubbard system*, Science, 6. Dec 2018 DOI:10.1126/ science.aat4134
- Grove-Rasmussen, K., Steffensen, G., Jellinggaard, A., Madsen, M. H., Žitko, Rok, Paaske, J., Nygård, J. Yu-Shiba-Rusinov screening of spins in double quantum dots. *Nature communications*, ISSN 2041-1723, 2018, vol. 9, str. 2376-1-2376-6, doi: 10.1038/s41467-018-04683-x. [COBISS.SI-ID 31479335]

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

We have been involved in the elucidation of charge regulation in colloid and biophysical systems. We have formulated a new theory of charge regulation in complex colloid solutions, composed of macroions with dissociable moieties (e.g., proteins), which generalizes all the previous attempts at understanding the colloidal solutions of macroions. We have analysed the statistical properties of active charged particles in the correlation effects in electrostatic interactions of anisotropic macromolecules. We have also studied the role of electrostatic interactions in the elasticity and shape of viral capsids.

We started studying configurations of particles on the surface of a sphere, interacting through a long-ranged dipolar interaction. In the scope of this work, we managed to generalize the classification of hyperuniform configurations of particles to the distributions of particles on the sphere.

We formulated a new statistical description of polymer nematics, which generalizes and consistently describes the Mayer-de Gennes conservation law. Also studied were the effects of chiral doping on phase transitions in achiral smectics. In the systems where interlayer interactions favour antichiral structures, the chiral structure is still stable at high enough temperatures. We investigated the properties of liquid-crystalline phases formed by bent dimers. A confined twist-bent nematic phase was shown to spontaneously form a polarization diffraction grating. By using the soft X-ray resonant scattering at the carbon K-edge we studied smectic phases formed by achiral bent dimers.

With atomistic modelling approaches we studied the thermodynamics of small solutes in thermos-responsive hydrogels, which are important for many applications of soft functional materials. We examined the phase diagram of soft colloidal particles described by the liquid-drop model, showing that it is very rich and that it includes several non-close-packed crystal lattices.

We developed a vertex model of an epithelial tissue characterized by so-called active topological transformations that fluidize the tissue. Using this model, we studied the viscoelastic response of the tissue. We also derived a continuum theory of the response, which nicely agrees with the numerical results.

### Some outstanding publication in the past three years

We studied the absorption of molecules in thermos-responsive hydrogels

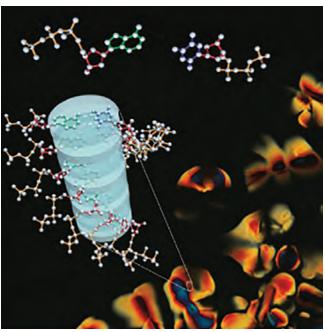


Figure 3: Schematic self-assembly of monomucleotide triphosphates into a DNA analogue with an absent phosphate backbone. Image courtesy of Tommaso P. Fraccia and Marco Todisco (University of Milan, Milan).

1. Šiber, Antonio, Ziherl, Primož. *Cellular patterns*. Boca Raton: CRC Press, Taylor & Francis, cop. 2018. XIII, 263 str., ilustr. ISBN 978-1-4822-5961-2. [COBISS.SI-ID 31043111]



2. Vaupotič, Nataša, Ali, Muhammad, Majewski, Pawel W., Gorecka, Ewa, Pociecha, Damian, Polarization Gratings Spontaneously Formed from a Helical Twist-Bend Nematic Phase, ChemPhysChem : a European journal of chemical physics and physical chemistry, ISSN 1439-4235 2018 (2018) 19, 2566-2571, doi: 10.1002/cphc.201800360. [COBISS.SI-ID 31667751].

### Organization of conferences, congresses and meetings

- 1. Correlated Electron systems in, near, and far from equilibrium, Ljubljana, Slovenia, 6.-8. 6. 2018
- Nonequilibrium Quantum Dynamics and Relaxation Phenomena in Many Body Systems, Krvavec, Slovenia, 16.-19. 12. 2018

### Awards and appointments

- 1. Prof. Saša Prelovšek Komelj: *Zois certificate of recognition* awarded by Republic of Slovenia for important achievements in theoretical particle physics
- Prof. Saša Prelovšek Komelj: *Excellent in science 2018* awarded by Slovenian Research Agency ARRS for most important achievements (10 achievements in a given year are chosen for natural sciences) awarded achievement: *Pion-nucleon scattering in the Roper channel from lattice QCD*, Physical Review D 95 (2017) 014510, C.B. Lang, L. Leskovec, M. Padmanath in S. Prelovsek
- 3. Prof. Rudolf Podgornik, Publons Peer Review Award for the year 2018 for reviewing manuscripts submitted to scientific journals. His reviewing work was also recognized by the American Chemical Society (Washington, DC, USA) as Marsha I. Lester, the editor of The Journal of Chemical Physics (Melville, NY, USA), mentioned him as one of the best reviewers of the journal.
- 4. Prof. Primož Ziherl, Advisor of the Year award for the year 2018 awarded by the Young Academy (Ljubljana).

## INTERNATIONAL PROJECTS

- 1. COST CA15108; Connecting Insights in Fundamental Physics (FUNDAMENTALCONNECTIONS) Prof. Jernej Fesel Kamenik
- Cost Office
- COST CA16201; Unraveling New Physics at the LHC through the Precision Frontier Asst. Prof. Miha Nemevšek Cost Office
- COST CA17139; European Topology Interdisciplinary Action Dr. Anže Lošdorfer Božič Cost Association Aisbl
- H2O20 ITN COLLDENSE; Hybrid Colloidal Systems with Designed Response Prof. Primož Ziherl
- European Commission 5. Relaxation Dynamics in Correlated Systems With Multiple Degrees of Freedom Prof. Janez Bonča
- Slovenian Research Agency
  Tools for Studying Systems with Extreme Correlations Asst. Prof. Rok Žitko
- Asser From Research Agency
   The Flavor of the Invisible Universe
- Asst. Prof. Nejc Košnik Slovenian Research Agency
- New Searches for Physics Beyond the Standard Model Prof. Jernej Fesel Kamenik Slovenian Research Agency

### **RESEARCH PROGRAMS**

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

## R & D GRANTS AND CONTRACTS

- Thermodynamics of dissipative nanosystems Dr. Iure Kokali
- 2. Orientational Interactions in a Generalized Thomson Problem: Dipole-Stabilized Spherical Nanocontainers
- Dr. Anže Lošdorfer Božič
- The many-impurity problem Asst. Prof. Rok Žitko
- Asst. 110. Rok 2000
   New physics implications of scalar resonances at the LHC Prof. Jernej Fesel Kamenik
- High-resolution optical magnetometry with cold cesium atoms Asst. Prof. Rok Žitko
- 6. Financing of projects visits at the Slovenian higher education institutions Asst. Prof. Jure Zupan
- Javni štipendijski, razvojni, invalidski in preživninski sklad Republike Slovenije 7. Financing of projects visits at the Slovenian higher education institutions Dr. Timon Mede

Javni štipendijski, razvojni, invalidski in preživninski sklad Republike Slovenije

## VISITORS FROM ABROAD

- 1. Dr. Kazuhiro Seki, SISSA, Trieste, Italy, 15.-17. 1. 2018
- 2. Dr. Alessio Maiezza, Institute Ruđer Bošković, Zagreb, Croatia, 15.-17. 1. 2018
- 3. Dr. Diptimoy Ghosh, ICTP, Trieste, Italy, 25.-26. 1. 2018
- Prof. Dr. Ilja Doršner, University of Split, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, Split, Croatia, 2.-14. 2., 20.-30. 4., 17.-23. 6., 25.-27. 7. 2018
- 5. Dr. Olcyr Sumensari, University of Padova, Padova, Italy, 5.-10. 2. 2018
- Juan Carlos Vasquez Carmona, Federico Santa María Technical University, Valparaíso, Chile, 16. 2.-1. 3. 2018
- 7. Prof. Dr. Duncan Haldane, Princeton University, Princeton, New Jersey, USA, 19.-
- 23. 3. 2018 8 Dr. Barry Dillor
- 8. Dr. Barry Dillon
- Prof. Dr. Mikhail Kiselev, ICTP, Trieste, Italy, 9-10. 4. 2018
   Dr. Zhang Yicheng, Pennsylvania State University, USA, 26, 5-10. 8.
- Dr. Zhang Yicheng, Pennsylvania State University, USA, 26. 5.-10. 8. 2018
   Dr. Slaven Barišić, Institut za fiziko, Zagreb, Croatia, 22. 5. 2018
- Dr. Staven Bartsic, Insulut za nziko, Zagreb, Groatta, 22. 5. 2018
   Dr. Huseyin Bahtiyar, Yildiz Technical University, Istanbul, Turkey, 1. 10.-31. 12. 2018
- Dr. Huseyin Banuyar, Yudiz Technical University, Istanbul, Turkey, I. 10.-51, 12, 20
   Dr. Minjae Kim, Ecole Polytechnique, Paris, France, 3.-5, 7, 2018
- Dr. Kfir Blum, Weizmann Institute, Rehovot, Israel, 8.-11. 7. 2018
- Prof. Dr. Geoff Rodgers, University of Brunel, London, Great Britain, 17.-22. 7. 2018

- Dr. Fagner Correia, Technical University of Dortmund, Dortmund, Germany, 20.-27. 8. 2018
- 17. Dr. Julio Leite, Universidade Federal do ABC, Sao Paulo, Brazil, 24. 8. 2018
- 18. Dr. Darko Tanasković, Institut za fiziko, Belgrade, Serbia, 29. 8.-1. 9. 2018
- 19. Dr. Jakša Vučičević, Institut za fiziko, Belgrade, Serbia, 29. 8.-1. 9. 2018
- 20. Prof. Dr. Anibar Karan, Institute of Mathematical Sciences, Chennai, India, 9.-
- 14. 9. 2018
- Prof. Dr. Deepak Dhar, Indian Institute of Science, Education and Research, Pune, India, 4.-6, 9, 2018
- 22. Dr. Gerardo Aldazabal, ICTP, Trieste, Italy, 27.-28. 9. 2018

### STAFF

#### Researchers

- 1. Asst. Prof. Milan Ambrožič
- 2. Prof. Borut Bajc
- 3. Dr. Damir Becirevic
- 4. Prof. Janez Bonča\*
- Prof. Mojca Čepič\*
- 6. Dr. Barry Michael Dillon
- 7. Dr. Ilja Doršner
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- 9. Prof. Jernej Fesel Kamenik
- 10. Dr. Matej Kanduč
- 11. Asst. Prof. Jure Kokalj\*
- 12. Asst. Prof. Nejc Košnik
- 13. Dr. Rajmund Krivec
- 14. Dr. Anže Lošdorfer Božič
- 15. Asst. Prof. Jernej Mravlje
- 16. Asst. Prof. Miha Nemevšek
- 17. Prof. Rudolf Podgornik\*
- 18. Prof. Peter Prelovšek
- 19. Prof. Saša Prelovšek Komelj
- 20. Prof. Anton Ramšak\*
- 21. Asst. Prof. Tomaž Rejec\*
- 22. Dr. Antonio Šiber
- 23. Prof. Bosiljka Tadić
- 24. Prof. Nataša Vaupotič\*
- 25. Asst. Prof. Lev Vidmar, 01.10.18, transferred to Department F7

- 23. Dr. Huseyin Bahtiyar, Yildiz Technical University, Istanbul, Turkey, 1. 10.-31. 12. 2018
- 24. Prof. Dr. Adrian Feiguin, Northeastern University, Boston, USA, 15.-17. 10. 2018
- 25. Dr. Joichiro Nakakura, University of Tokyo, Japan, 4.-10. 11. 2018
- Prof. Dr. Damir Bečirević, Laboratoire de Physique Theorique d'Orsay, Univ. Paris-Sud, France, 12.-23. 11. 2018
- Prof. Dr. Masayuki Imai, Ochanomizu University, Tokyo, Japan, 25.-28. 11. 2018
- Prof. Dr. Gia Dvali, Arnold Sommerfeld Center, Ludwig-Maximilians-Universität, Max-Planck-Institut für Physik, München, Germany, Center for Cosmology and Particle Physics, Department of Physics, New York University, New York, USA, 9-11. 12. 2018
- 29. Dr. Lucas Hackl, Max-Planck Institute, Garching, Germany, 10.-13. 12. 2018
- 26. Prof. Primož Ziherl\* 27. Asst. Prof. Jure Zupan 28. Asst. Prof. Rok Žitko Postdoctoral associates 29. Dr. Monalisa Patra 30. Dr. Maja Pečar\* 31. Dr. Jan Skolimowski 32. Dr. Tjaša Švelc Kebe, left 01.07.18 33. Dr. Šaša Ziherl\* Postgraduates 34. Andreas Kyriakos Doukas, B. Sc., left 15.06.18 35. Darius Alexander Faroughy Carias, B. Sc. 36. Victor Francisco Guada Escalona, B. Sc. 37. Alen Horvat, B. Sc., left 01.05.18 38. Jan Rozman, B. Sc. 39. Urša Skerbiš Štok, B. Sc. 40. Aleks Smolkovič, B. Sc. 41. Jan Šuntajs, B. Sc. 42. Lara Ulčakar, B. Sc.
- Technical and administrative staff 43. Nevenka Hauschild

Note:

\* part-time JSI member

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# DEPARTMENT OF LOW AND **MEDIUM ENERGY PHYSICS**

The Department of Low and Medium Energy Physics is engaged in research in the field of atomic and nuclear physics. Knowledge acquired in basic research is exploited for numerous applications, including radiological monitoring of the environment, in material research, fusion, biology, energy storage, medicine, pharmacology, environment and archaeometry. Research is executed using our own experimental equipment, consisting of an 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 2018 we have continued our work at the three-spectrometer facility of the Mainz Microtron (MAMI) with measurements of electron scattering using transversely polarized electrons, with production running on <sup>90</sup>Zr nuclei. These studies represent an attempt to understand the fundamental symmetries of hadronic physics, exploiting observables sensitive to transverse polarization instead of the usual longitudinal polarization that probes **Prof. Primož Pelicon** the strangeness content of the nucleon. Our previous study of the Q2-dependence of the beam-normal single spin

asymmetry for elastic scattering off <sup>12</sup>C has been published (Esser et al, Phys. Rev. Lett. 2018). We have also concluded the analysis of components of polarization transfer to a proton bound in a deuteron, measured by quasi-elastic electron scattering, as well as the analysis of the equivalent process on carbon in terms of virtuality (Izraeli et al., Phys. Lett. B 2018). Further effort was invested in commissioning the gas-jet target intended for background-free measurements of nucleon form-factors both by means of the standard technique and by exploiting the method based on initial-state radiation (ISR): the latter depends on virtually perfect knowledge of the radiative tail of the elastic peak to access the proton charge form factor at extremely small momentum transfers, and offers a distinct approach to addressing the famed "proton radius puzzle". We have also worked on the commissioning of the new, multi-purpose neutron polarimeter.

Our work at the Thomas Jefferson National Accelerator Facility (Jefferson Lab) has been focused on running a comprehensive group of experiments using a tritium target. This effort has given us a unique opportunity to explore <sup>3</sup>H and its mirror nucleus of <sup>3</sup>He, and thereby impose severe constraints on state-of-the-art theories of nuclear many-body systems, in particular relating to the aspect of isospin symmetry. The experiment group consisted of:



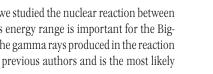
Figure 1: Measurements of gamma radioactivity in situ with a highpurity germanium spectrometer within the environmental monitoring of the radioactivity in the enevironment

- investigating the deep inelastic scattering off <sup>3</sup>H and <sup>3</sup>He to measure the EMC effect for both nuclei and to determine the ratio of the neutron-to-proton inelastic structure functions, as well as probing the ratio of the down to up quark distributions in the nucleon;
- a precision test of the isospin dependence of two-nucleon short-range correlations in <sup>3</sup>H and 3He;
- quasi-elastic scattering to measure the proton and neutron momentum distributions in <sup>3</sup>H and <sup>3</sup>He, trying to demonstrate that the minority (protons in <sup>3</sup>H) have an average kinetic energy higher than the majority (protons in <sup>3</sup>He); exclusive kaon electroproduction on <sup>3</sup>H.

The beam-time was successful, and all the above data analyses are now underway. We have published papers on our previous work on proton elastic form factors during high-momentum transfers (Puckett et al, Nucl. Instr. Meth. A 2018), on three-nucleon short-range correlations (Ye et al, Phys. Rev. C 2018) and inclusive cross-section measurements on Ti nuclei (Dai et al, Phys. Rev. C 2018).

With the Tandetron accelerator at the Microanalytical Center in 2018 we studied the nuclear reaction between protons and deuterons in the energy range between 70 and 320 keV. This energy range is important for the Big-Bang nucleosynthesis, which created the lightest elements. We found that the gamma rays produced in the reaction possess a large angular anisotropy, which was not taken into account by previous authors and is the most likely

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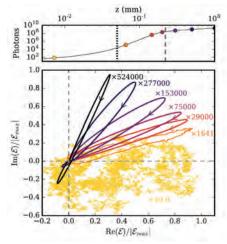


Figure 2: Number of photons (up) and the phase of the electric field (bottom), emmited at the excitation with a 100 fs light pulse with intensity of  $4 \times 10^{14}$  W/cm<sup>2</sup> as a function of the helium target thickness at a pressure of 30 Pa (Krušič et al, Phys. Rev. A 2018).

reason for the discrepancy in their measurements with the latest ab-initio theory of nuclear reactions. Our measurements agree with the aforementioned theory. The work has been submitted for publication in European Physical Journal A and will be included in the PhD thesis of young researcher Isabela Tišma.

We engaged in collaborative activities at the international nuclear research centre FAIR. The first 12 segments of the CALIFA detector have been acquired and their assembly started. Computer simulations of the BGO veto detectors for the DEGAS system were completed and yielded the geometrical configurations for the SiPM sensor positions. The voltage stabilization and precision timing for the electrostatic lenses of the time-of-flight ion mass spectrometer Super-FRS has been designed and its assembly started.

Members of the Infrastructure Group for Ionizing Radiation Measurements were involved in research fields related to ionising radiation and nuclear physics. In addition, they were conducting activities in 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 the radioactivity in fodder, central radioactive waste repository radiological monitoring, monitoring of the radioactivity in drinking water, material characterizations, calibrations of the radiation gauges and the measurements of the personal and environmental doses by thermo-luminescent dosimeters. All the listed activities are accredited according the standard SIST EN ISO/IEC 17025.

In 2018 we continued our intensive collaboration with the Metrology Institute of the Republic of Slovenia (MIRS). As a designated institution and as the holder of the national standard for the field of ionizing radiation, we continued the activities on the project within the European Metrology Research Programme (EMRP) "Preparedness – Metrology for mobile detection of ionising radiation following a nuclear or radiological incident". Within this project, we are developing and upgrading the novel gamma-radiation hotspot locator available at the JSI and based on CsI detectors with an angular sensitivity based on the AISense Gamma monitor, to be mountable on an unmanned helicopter, in collaboration with UPC, Barcelona, Spain,.

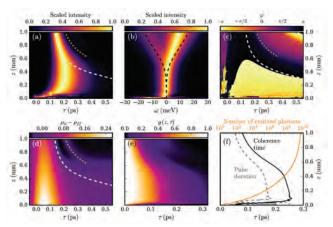


Figure 3: Evolution of the temporal (a) and spectral intensity profile of the emitted field (b), the temporal profile of the phase of the emittedfield (c), population inversion (d), and autocorrelation function of the emitted field (e) in the target after a single extreme ultraviolet light pump pulse from a free-electron laser (Krušič in sod., accepted for publication in Phys. Rev. A).

In 2018, the members of the department started to work on a new project ENRAS (ENsuring RAdiation Safety) in the framework of the Cooperation Programme Interreg V-A Slovenia-Croatia 2014-2020. The project involves IJS (leading partner), Institute for Medical Research and Occupational Health - IMI (project partner 1), Zagreb, Croatia and Fire-fighter Association of Slovenia - GZS (project partner 2). The aim of the project is to develop cross-border cooperation in the field of safety (civil protection) in the event of a nuclear or radiological emergency. Members of the Infrastructure Group also took part in regular drills and special tasks with the radiological mobile unit ELME.

In 2018 we have published three papers from the field of theoretical atomic physics in Physical Review A, where we have considered for the first time the interaction of atoms with intense XUV light. The first paper deals with the phenomenon of superfluorescence suggesting to measure time dependence of  $2 \, ^{1}P \rightarrow 2 \, 1S$  radiation emitted in the decay of the  $2 \, ^{1}P$  state in helium, which is prepared by the intense XVU laser pulse (Figure 2). This is a prototypical system, where the phenomenon appears in the simplest three-level scheme. We published a detailed simulation showing the time dependence of the fluorescence developing from spontaneous emission, superfluorescence towards the self-amplified spontaneous emission (*Krušič et al, Phys. Rev A 2018*). The second paper studies the form

of the Beer-Lambert law in the time domain (Žitnik *et al*, *Phys. Rev A 2018*). It turns out that the time dependence of the light pulse at the target exit can be expanded into the sum of the weighted characteristic contributions. These can be calculated in advance and depend on the temporal dependence of the entrance pulse and the nature of the resonant states. The third paper presents the calculated two-photon absorption cross-section of helium in the broad range of photon energies showing an enormous enhancement of the cross-section in the region of the core resonances, i.e., when the energy of the incoming photons matches a dipole allowed transition in the helium ion, for example, He<sup>+</sup> n=2 $\rightarrow$ n=1 (*Mihelič et al*, *Phys. Rev. A 2018*). An open question remains as to how to experimentally isolate this effect, because it is difficult to separate the fluorescence signal from the one originating in the sequential photo-absorption. In 2018 we analysed and published the results of experiments that were performed at MaxLab in Lund, Sweden, together with researchers from Oulu University in Finland. We have measured for the first time the two-dimensional maps of the resonant Auger decay in coincidence with the selected ionic species that appear in the final state of molecular dissociation, triggered by photoexcitation (*Kokkonen et al, Jour. Chem. Phys. 2018*). It turned out that the (Cl)L-VV Auger spectra significantly differ in chloromethanes, although in all these cases the chlorine atom is bound to the carbon (Figure). This means that the spectrum does not depend solely on the initial dissociation dynamics, but also on differences in the charge redistribution in different molecules, triggered by dissociation.

We participated in synchrotron experiments at Soleil, Paris, where we aimed to observe an atomic signal from thin layers deposited on thin wires, placed in the field of detection of the magnetic bottle spectrometer. Another experimental attempt was concerned with electron retardation to improve the spectral resolution of the magnetic bottle. We took part in the experiment with high-harmonic generation in the Laboratory for Quantum Optics at the University of Nova Gorica, where AC Stark maps of the ion yield were measured upon the coupling of a pair short-lived states with an IR laser light pulse. We prepared an experimental project at the free electron laser FERMI, involving collaborators from France and dealing with a coherent control of Auger emission. In the frame of the EMRP "Aeromet" project we were concerned with the characterization of the simple optical dust detectors and their comparison with the results of the more sophisticated instruments. For this we attended the measurement campaign in Cassino, Italy. The ongoing comparative analysis shows that a good knowledge of the operational parameters of the simple optical counters in conjunction with the data acquired by the sophisticated device can significantly broaden the temporal and spatial range coverages of dust monitoring without significant additional costs.

In the field of high-energy-resolution x-ray spectroscopy we have successfully performed *in-operando* sulphur EXAFS measurements from a cathode of a magnesium sulphur (Mg-S) battery during discharge. The experiment took place at the ID26 beamline of the ESRF synchrotron in

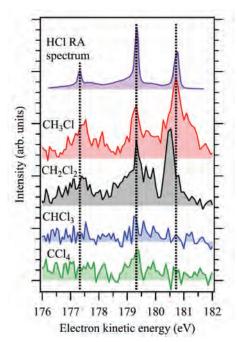


Figure 4: Resonant Auger spectra Cl2p-VV, measured in coincidence with Cl<sup>+</sup> ions at the decay of photoexcited resonance (Cl)2p1 $\sigma^*$  for all four molecules of chlorometanes (Kokkonen et al, Jour. Chem. Phys. 2018).

collaboration with the group from the National Institute of Chemistry in Ljubljana. In order to remove the sulphate signal from the electrolyte, a sulphur-free electrolyte was used in the battery to record a long enough energy range above the sulphur K edge required for EXAFS analysis. This experiment will provide precise quantitative structural

information, including the local coordination of S, on each of the characteristic magnesium sulphur compounds build up electrochemically during the battery's operation and will complement our previous characterization of sulphur within a Mg-S battery using RIXS/XAS measurements. Besides synchrotron measurements, we have also recorded in our home laboratory proton-induced high-energy-resolution sulphur K $\alpha$  and K $\beta$  x-ray emission spectra from several cathodes of Li-S batteries stopped at different points during discharge. These measurements will demonstrate the feasibility to characterize sulphur compounds build electrochemically within the battery cathode, which is currently restricted to synchrotron studies, also in a smaller laboratory using a laboratory excitation source. In the field of high-energy-resolution PIXE spectroscopy we have continued our collaboration with the group from University of Guelph, Ontario, Canada, and recorded KL multiple ionization satellites in the K X-ray spectra of pure Ti and several titanium binary oxides induced in collisions with MeV alpha particles. These results will expand further the existing He-induced multiple ionization satellites database, which will be used to improve the accuracy of the PIXE analysis using alpha particle beams, including the PIXE mode of the alpha particle X-ray spectrometers (APXS) installed in the Mars rover Curiosity.

During 2018, the results of the  $L_3^{-}M_{4,5}$  resonant inelastic x-ray scattering (RIXS) measurements on Ag within  $Ag_xMo_9Se_{11}$  (x=3.4 and 3.9) polycrystalline samples were published (*Butorin et al*, *ACSAppl. Ener. Mat. 2018*). The experimental data were used to study the effect of Ag doping

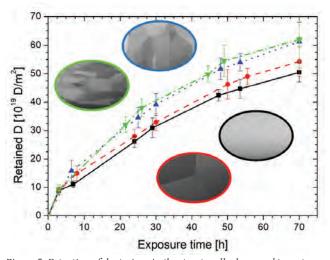


Figure 5: Retention of deuterium in the structurally damaged tungsten layer as a function of exposure time for four studied samples as derived from nuclear reaction analysis by <sup>3</sup>He ions. Images obtained on the surface of the samples using a scanning electron microscope are also inserted in the graph. The colour line around the image also denotes the data points in the graph. (Pečovnik et al., accepted for publ. in Jour. Nucl. Mat.).

on the electronic structure of  $Ag_x Mo_9 Se_{11}$  as a potential material for thermoelectric applications. K X-ray spectra of Si induced in collisions with 3-5 MeV He ions, performed at the Microanalytical center, were used to extract the data on KL<sup>n</sup> multiple ionization satellites (*Heirwegh et al, Nucl. Instr. Meth. B 2018*). High-energy-resolution PIXE spectroscopy has been used successfully to perform the chemical speciation of sulphur in a biological tissue

(*Kavčič et al, Nucl. Instr. Meth. B 2018*). Measurements of the K $\alpha$  emission line were used to determine the ratio of S<sup>6+</sup>/S<sup>2-</sup> species within the tissue and the K $\beta$  emission spectrum confirmed the transformation of sulphur from the uptake sulphate form, to fully reduced sulphur within large sulphur-containing organic molecules. In collaboration with the University of Fribourg, Switzerland, we have published the results on the hypersatellite x-ray decay of 3*d* hollow K-shell atoms produced in collisions with heavy ions (*Maillard et al, Phys. Rev. A 2018*).

In 2018, we continued with research in fusion, coordinated by the EUROfusion Consortium and carried out within the work package on "Preparation of efficient Plasma-Facing Component (PFC) operation for ITER and

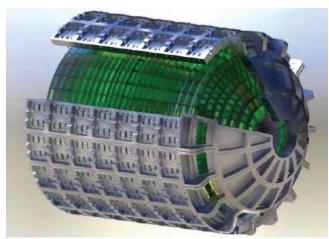


Figure 6: Detector CALIFA of the NUSTAR collaboration at FAIR is concepted as a scintillation calorimeter for gamma rays and charged particles. In 2018 we started to build 12 segments for the detector system.

DEMO". Hydrogen-isotope interactions with materials play a crucial role in fusion research as the tritium inventory needs to be controlled inside a future reactor and maintained below specific limits for safe and fuel-efficient operation. Within the expected operational duty cycles the displacement damage from irradiation by energetic 14.1 MeV neutrons produced by the deuterium-tritium fusion reaction (D + T  $\rightarrow$  He (3.5 MeV) + neutron (14.1 MeV)) is anticipated to be a few displacements per atom per year, adding challenges to the material choice. Tungsten and tungsten alloys are considered to be the most suitable materials for plasma-facing components in future fusion reactors such as DEMO. For this reason, a major focus of our research is the study of hydrogen-isotope retention in tungsten material. Lattice defects, produced due to irradiation by 14 MeV neutrons and ions from the plasma, act as trapping sites for hydrogen isotopes with a high de-trapping energy, as compared to the energy of the diffusion of hydrogen in tungsten. In order to study the influence of the neutron irradiation of materials on fuel retention, high-energy W ions produced by MV accelerators are used to produce displacement damage, which mimics the damage created by neutrons very well.

We have focused on two subjects in this year. The first was to study the influence of grain size on deuterium transport and retention in tungsten. For this purpose, an experiment was carried out on three polycrystalline tungsten samples with different grain sizes and a single-crystal sample with surface orientation <100> that were first damaged by 20-MeV energy W ions. After damaging, the samples were exposed to a  $4 \times 10^{18}$  m<sup>-2</sup>s<sup>-1</sup> flux of deuterium atoms at 600 K for 70 h. The increase of D retention is shown as a function of exposure time in Figure 1 for the studied samples. We have observed different D uptakes for the different grain sizes was modelled by changing the effective height of the potential barrier for deuterium atoms to enter into the bulk. We managed to successfully describe the transport of deuterium into the bulk of tungsten, showing that a larger surface density of grain boundaries provides more access for the diffusion of D into the material (*Pečovnik et al, accepted for publ. in Jour. Nucl. Mat.*).

The second subject was continuing the study of the influence of D's presence on the defect production by simultaneous W-ion damaging and D-atom exposure. The first experimental results were published in Markelj et

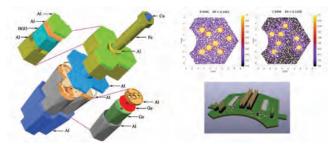


Figure 7: Optimization of the detection system DEGAS in the FAIR/ NUSTAR with simulation tools. The simulation provided the positioning for optimal light collection of a limited number of silicon photomultipliers.

al. Nucl. Mater. Energy 12 (2017) 169. This year we performed modelling of the experimental data in collaboration with CEA, France (*Hodille et al. Nucl. Fusion 2019*). Modelling of the measured deuterium depth profiles and thermal-desorption spectra for different irradiation temperatures was performed by the MHIMS (migration of hydrogen isotopes in materials) code. A model of trap creation due to tungsten-ion irradiation during the deuterium-atom exposures was implemented. The experiments give an unambiguous proof that the presence of deuterium increases the overall trap density. The modelling reveals that there are two traps with de-trapping energies of 1.83 eV and 2.10 eV that are affected differently by the temperature and the presence of deuterium. The concentration of the low-energy trap is significantly higher in the case of simultaneous exposure as compared to the sequential exposure, especially at high temperature (2.2 times higher at 1000 K). The concentration of the high-energy trap is only weakly affected by the presence of hydrogen. In this year we have

also upgraded the experiment by studying the influence of D presence on defect production by simultaneous W-ion damaging and D-ion exposure, where the even larger effect of defect stabilization is observed.

The tandem accelerator at the Jožef Stefan Institute **operated** successfully in 2018 and provided over 3500 hours to users from the fields of fusion, biology, medicine, nuclear astrophysics, materials and energy research. Further

instrumental developments were dedicated to the MeV-SIMS technique, where we achieve sub-micrometre lateral resolution on the thin biological tissue slices. Within a new research project of the Slovenian Research Agency titled "Molecular imaging inside the cell" we started an upgrade of the linear Time-Of-Flight mass spectrometer into the reflectron configuration.

Intense applied research was undergoing at the high-energy focused ion beam, where micro-PIXE and MeV-SIMS techniques were used for studies in biology, medicine and related research fields. Research in biology was undergoing in close collaboration with the Biotechnical Faculty of the University of Ljubljana. We continued the collaboration with Jagiellonian University in Krakow, where we determined the metal stoichiometry in synthetic proteins (Malay et al, accepted for publ. in Nature). The interaction of nano zero-valent iron with roots of maize was studied in collaboration with the Czech University of Life Sciences Prague (Wu et al, Env. Sci. Tech. 2018). Elemental profiles of Scots pine needles were studied in collaboration with Vilnius Gediminas Technical University, Lithuania (Pongrac et al, Trees, 2018). We started to work on several new research projects, including the EU MC postdoctoral project of dr. Esther Punzon Quijorna, titled "TissueMaps", dedicated to the elemental imaging of human tissue, providing clinical therapy support and the development of new diagnostics. Clinical cases of hip-prosthesis failures were studied in collaboration with University Clinical Centre Maribor by complementing the standard tissue pathology procedures with elemental-sensitive microscopy micro-PIXE

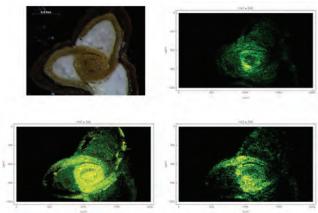


Figure 8: Cross-section of a buckwheat grain under optical microscope (upper left) and the distribution of the molecular ions with the masses of 104, 398 and 786, measured with MeV-SIMS. All three molecular ions are mostly present in the kotyledon (Jenčič et al., unpublished).

and several other modalities of advanced microscopies. We started to work on the physiology studies of buckwheat within a new research project of the Slovenian research agency "Locally grown buckwheat grain for the production of high-quality food products". Here, we applied molecular imaging with MeV-SIMS to resolve the molecular distributions in buckwheat seeds, with a focus on the distribution of the anti-oxidant molecules rutin and quercitrin.

We continued with the instrumental improvements at the beamline with the in-air proton beam. In parallel, intense research work was executed with the in-air PIXE at the field of archaeometry, as well as the study of the ancient counterfeit coins and the elemental fingerprints of coffee within the Coordinated research project of the IAEA titled 'Enhancing Nuclear Analytical Techniques to Meet the Needs of Forensic Science'.

# Organization of conferences, congresses and meetings

- 1. WG 3 MODARIA, 7-10 May 2018, Ljubljana
- 2. ISO/TC 201/SC10, 24 June 2018, Ljubljana
- 3. EXRS 2018, 25-29 June 2018, Ljubljana

# INTERNATIONAL PROJECTS

- H2020 TRANSAT; TRANSversal Actions for Tritium Asst. Prof. Sabina Markelj European Commission
- 2. Services
- Branko Vodenik, M. Sc. 3. Calibrations
- Matjaž Mihelič, M. Sc. 4 TLD Dosimetria
- Boštjan Črnič 5. FAIR Detectors
- Prof. Matej Lipoglavšek Gsi Helmholtzzentrum
- EMPIR; Preparedness Metrology for Mobile Detection of Ionising Radiation Following a Nuclear or Radiological Incident Dr. Teori Petrovičá
- Dr. Toni Petrovič Euramet E.v.
- 7. EMPIR; AEROMET Aerosol Metrology for Atmospheric Science and Air Quality Prof. Matjaž Žitnik
- Euramet E.v.
- Training Fees for Mr. Eyakifama Hazou Asst. Prof. Benjamin Zorko IAEA - International Atomic Energy Agency
- 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

Asst. Prof. Klemen Bučar

- IAEA International Atomic Energy Agency
- 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
- COST CA16117 ChETEC; Chemical Elements as Tracers of the Evolution of the Cosmos Prof. Matej Lipoglavšek
- Cost Office 12. Training Fees for Mr. Andrii Kholodyuk, STEP Asst. Prof. Benjamin Zorko
- Ictp Centro Internazionale Di Fisica Teorica
- Enhancing Nuclear Analytical Techniques to Meet the Needs of Forensic Sciences; Forensics with Nuclear Methods: Art and Food Forgery, Drugs in Hair Prof. Primož Pelicon
- IAEA International Atomic Energy Agency
- Training Fees for IAEA"s Fellow Mrs. Margarita Ginovska (SV/MAK2007-1702343), 28.1.2018-3.2.2018
- Asst. Prof. Benjamin Zorko
- IAEA International Atomic Energy Agency 15. COST CA18130; European Network for Chemical Elemental Analysis by Total Reflection
  - X-Ray Fluorescence
- Dr. Marijan Nečemer
- Cost Office
- 16. H2020 CONCERT; European Joint Programme for the Integration of Radiation Protection Research



Asst. Prof. Benjamin Zorko European Commission

- H2020-EUROfusion-Plasma Facing Components-1-IPH-FU, EUROFUSION Asst. Prof. Sabina Markelj
- European Commission 18. H2020 EUROfusion - Education-ED-FU Prof. Primož Pelicon
- European Commission
- H2020 EUROfusion Medium Size Tokamak Campaigns-MST1-FU Mitja Kelemen
- European Commission
- H2020 TissueMaps Elemental Imaging of Human Tissue: Clinical Therapy Support and Development of New Diagnostics Prof. Primož Pelicon
- European Commission
- Electron Scattering Studies of 3H/3He Mirror Nuclei Prof. Simon Širca Slovenian Research Agency
- Gamma Spectrometric Determination of Low Level Activity of Low-Energetic Radionuclides in Complexs Samples Asst. Prof. Benjamin Zorko
- Slovenian Research Agency
- WG3 MODARIA II, Third Technical Meeting of MODARIA II Asst. Prof. Benjamin Zorko Slovenian Research Agency
- Study of Weak Charge Distributions with Precision Parity-Violating Measurements Dr. Miha Mihovilovič
- Slovenian Research Agency 25. Electrochemical Reactions in Organic-Metal Batteries Studied by X-Ray Raman Spectroscopy Asst. Prof. Matjaž Kavčič
  - Slovenian Research Agency

# RESEARCH PROGRAMS

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

# R & D GRANTS AND CONTRACTS

- 1. Triggering forbidden phenomena with twisted light and particles beams Prof. Matjaž Žitnik
- Redox active organic materials for electrical energy storage Asst. Prof. Matjaž Kavčič

# VISITORS FROM ABROAD

- Margarita Ginovska, Ss. Cyril and Methodius University, Skopje, Macedonia, 28 January - 3 February 2018
- 2. Andrii Kholodiuk, Institute for Safety Problems of NPP, Kiev, Ukraine, 12 February 12 May 2018
- 3. Prof. Dr. Jechiel Lichtenstadt, Tel Aviv University, Tel Aviv, Israel, 12–13 March 2018
- 4. Dr. Tim Vidmar, SCK-CEN, Mol, Belgium, 7-20 May 2018
- 5. Dr. Venkata Dasireddy, UKZN, Durban, South Africa, 3 April 28 May 2018
- Dr. Sebastijan Brezinšek, Institut für Plasmaphysik, Forschungszentrum, Jülich, Germany, 16–19 April 2018

- 3. Ionom of crop plants for safe and quality food production Prof. Katarina Vogel-mikuš
- Stable isotopes in the study of the impact of increasing CO2 levels on C and Hg cycling in coastal waters
   Partic Katanica Veral miluxă
- Prof. Katarina Vogel-mikuš 5. Three-dimensional distribution of mineral elements in plant leaves
- Asst. Prof. Paula Pongrac
- 6. Molecular imaging inside the cell
- Prof. Primož Pelicon7. Localy grown buckwheat grain for production of high quality food productsProf. Primož Pelicon
- 8. ENRAS: Ensuring Radiation S afety for First Responder Teams in Case of Radiological or Nuclear Accidents
  - Boštjan Črnič Government Office for Development and European Cohesion Policy
- BEST: Barley stress tolerance Prof. Primož Pelicon Ministry of Education, Science and Sport
  - . Different Analyses
  - Dr. Jasmina Kožar Logar
- 11. Irradiation and Analysis of Nano SiC Samples in the Year 2017 Asst. Prof. Benjamin Zorko
- National Nuclear Research Center 12. Support to the Quality Infrastructure in Serbia Denis Glavič Cindro, M. Sc.
- Physikalisch-technische Bundesanstalt (ptb) 3. EURAMET TC-Ionising Radiation (TC-IR) Annual Meeting 2019 and Working Meetings
- EURAME 11C-Ionising Radiation (1C-IR) Annual Meeting 2019 and working Meeting within EMPIR Projects Preparedness and DOSEtrace Denis Glavič Cindro, M. Sc.

# NEW CONTRACTS

- Determination of blocking temperature on two frozen liquid iron containing samples using Mössbauer spectroscopy Dr. Darko Hanžel
  - Lek d. d.
- Analyses of atmospheric releases in 2018 Asst. Prof. Benjamin Zorko Nuklearna Elektrarna Krško d. o. o.
- Off-site radiological monitoring of the Krško Nuclear Power Plant in 2018 and 2019 Asst. Prof. Benjamin Zorko
- Nuklearna Elektrarna Krško d. o. o. 4. Monitoring of radiaoactivity in drinking water in Republic of Slovenia in 2018 and 2019 Asst. Prof. Benjamin Zorko
- Ministry of HealthTesting of the geographical origin of fruits and vegetables using elemental composition and stable isotopes
  - Dr. Marijan Nečemer
- Ministry of Agriculture, Forestry and Food 6. Maintenance of radiological emergency preparedness 2018 Asst. Prof. Benjamin Zorko
- Nuklearna Elektrarna Krško d. o. o.
- Dr. Katja Magdić Košiček and Dr. Ivana Tucaković, IRB, Zagreb, Croatia, 7 September 2018
- Eyakifima Hazou, University of Lome, Lome, Togo, 10 September 8 December 2018
   Laura Péres Orosa, USC, Santiago de Compostela, Galicia, Spain, 2 September 2 December 2018
- Dr. Thomas Schwartz-Selinger, Max Planck Institute for Plasma Physics, Garching, Germany, 1–5 October 2018
- 11. Dr. Jelena Ajtić, University of Belgrade, Belgrade, Serbia, 18-19 December 2018

# STAFF

- Researchers
- 1. Prof. Iztok Arčon\*
- 2. Asst. Prof. Klemen Bučar
- Prof. Dean Cvetko\*
   Denis Glavič Cindro, M. Sc.
- Denis Giavic Cindro, M. Sc
   Dr. Darko Hanžel
- 6. Asst. Prof. Matjaž Kavčič

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9.

Dr. Jasmina Kožar Logar

Prof. Matej Lipoglavšek Asst. Prof. Sabina Markelj

10. Asst. Prof. Andrej Mihelič

13. Prof. Primož Pelicon, Head

11. Dr. Miha Mihovilovič

12. Dr. Marijan Nečemer

Annual Report 2018

14 Dr Toni Petrovič 15. Asst. Prof. Paula Pongrac 16. Prof. Simon Širca\* 17. Prof. Žiga Šmit\*, left 01.11.18 18. Asst. Prof. Matjaž Vencelj 19. Branko Vodenik, M. Sc. 20. Prof. Katarina Vogel-Mikuš\* 21. Asst. Prof. Benjamin Zorko 22. Prof. Matjaž Žitnik Postdoctoral associates 23. Dr. Tilen Brecelj 24. Dr. Boštjan Jenčič 25. Dr. Romana Krištof 26. Dr. Eva Menart\* 27. Esther Punzon Quijorna, B. Sc. 28. Dr. Jelena Vesić 29. Dr. Anže Založnik, left 01.09.18 Postgraduates

30. Žiga Barba, B. Sc.

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# ORIGINAL ARTICLE

- 1. S. M. Butorin, K. O. Kvashnina, M. Klintenberg, Matjaž Kavčič, Matjaž Žitnik, Klemen Bučar, P. Gougeon, P. Gall, C. Candolfi, B. Lenoir, "Effect of Ag doping on electronic structure of cluster compounds  $Ag_xMo_9Se_{11}$  (x = 3.4, 3.9)", *ACS applied energy materials*, 2018, **1**, 8, 4032-4039.
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- 5. Janvit Teržan, Petar Djinović, Janez Zavašnik, Iztok Arčon, Gregor Žerjav, Matjaž Spreitzer, Albin Pintar, "Alkali and earth alkali modified CuO<sub>x</sub>/SiO<sub>2</sub> catalysts for propylene partial oxidation: what determines the selectivity?", *Applied catalysis. B, Environmental*, 2018, 237, 214-227.
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31 Mateia Hrast B Sc. 32. Tim Kolar, B. Sc. 33. Špela Krušič. B. Sc 34. Matic Pečovnik, B. Sc. Isabela Tišma Technical officers 36. Boštian Črnič, B. Sc 37. Mitja Kelemen, B. Sc. Matjaž Mihelič, M. Sc. 39. Dr. Primož Vavpetič Technical and administrative staff 40. Drago Brodnik 41. Mojca Gantar 42. Sandi Gobec 43. Mirko Ribič, B. Sc. Note: \* part-time JSI member

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- 13. Francine Ilunga Kabeya, Paula Pongrac, Bastien Lange, Michel-Pierre Faucon, Johannes Teun van Elteren, Martin Šala, Vid Simon Šelih, Emilie Vanden Eeckhoudt, Nathalie Verbruggen, "Tolerance and accumulation of cobalt in three species of Haumaniastrum and the influence of copper", *Environmental and experimental botany*, 2018, **149**, 27-33.
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# PUBLISHED CONFERENCE CONTRIBUTION (INVITED LECTURE)

1. Katarina Vogel-Mikuš, Iztok Arčon, Peter Kump, Alojz Kodre, "Metal concentration and speciation in soil and plants by X-ray fluorescence and absorption spectrometry", In: Neža Finžgar (ed.), *Demonstration of innovative soil washing technology for removal of toxic metals from highly contaminated garden soil: proceedings of the conference*, 2018, 27-29.

# PUBLISHED CONFERENCE CONTRIBUTION

- Peter Kump, Katarina Vogel-Mikuš, "Quantification of 2D elemental distribution maps of intermediate-thick biological sections by low energy synchrotron μ-X-ray fluorescence spectrometry", In: 24th International Congress on X-Ray Optics and Microanalysis, 24-29 September 2017, Trieste, Italy, (Journal of instrumentation 13) 2018, 5, C05014.
- 2. Olena Pliekhova, Oleksii Pliekhov, Mattia Fanetti, Iztok Arčon, Nataša Novak Tušar, Urška Lavrenčič Štangar, "The effect of Zr loading on photocatalytic activity of Cu modified TiO<sub>2</sub>", In: Sixto Malato Rodríguez (ed.), Proceedings of the 10th European Meeting on Solar Chemistry and Photocatalysis: Environmental Applications [also] (SPEA10), Palacio de Exposiciones y Congresos, Cabo de Gata, Ciudad de Almería, Almería (SPAIN), June, 4th-8th 2018, 2018, 242-243.
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#### MENTORING

- 1. Tilen Brecelj, Measurement of in-medium modifications of proton formfactors: doctoral dissertation, Ljubljana, 2018 (mentor Simon Širca).
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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. In the applied research, different coatings are developed for the protection of tools for various production processes in industry.

For many years, the department has predominantly conducted research on coatings deposited by magnetron sputtering. This research has been conducted on a basic level, which includes the study of magnetron plasma, as well as in an applied manner; in this respect there is our important recent work on growth defects in thin films. Namely, these defects are a significant obstacle in the application of coatings. Indeed, one of the important subjects of the department's activities is dedicated to industrial applications, as we offer our coatings to the industrial partners within the Hard Coating Center. Our deposition of coatings on industrial tools has been predominantly performed using magnetron sputtering, accompanied to a minor extent using the older technique of thermionic arc evaporation.

this technique is well known as it uses a simple, reliable principle of coating deposition, but it has the drawback of a high density of the emitted microdroplets, which in turn increases the roughness of the deposited coatings. However, this phenomenon is interesting from the research point of view, especially from the perspective of our previous research on growth defects. Thus, we acquired a good tool for an additional, extended study of growth defects, and simultaneously also an additional piece of equipment for the implementation of new coatings for our industrial partners. Using different deposition techniques we are now able to deposit the following coatings: TiN, CrN, AlCrN, TiAlN (several Ti:Al stoichiometries), AlTiN-based nanolayer coatings and TiAlSiN-based nanocomposite coatings.

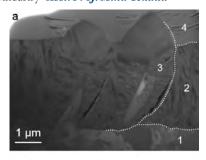
In the current year we made a systematic characterization of all the above-listed coatings prepared by different deposition procedures, and this will serve us as a reference for future work. Another step forward is the deposition of these coatings on standard endmills, which are being tested on a machine tool in collaboration with the Mechanical Engineering Faculty at the University of Ljubljana. In collaboration with some other partners we deposited perspective coatings on selected tools, and these were consequently tested by the partners in a semi-industrial environment. Within a well-established cooperation with the University of Novi Sad (Serbia) we conducted several advanced tribological experiments; afterwards these coatings were tested for the protection of aluminium die casting tools. Due to the complex conditions, these tools (punches) were previously nitrided and additionally polished. Using the TiAlN coating the lifetime of the tools improved by a factor of four. The protection of aluminium die-casting tools is one of the topics within the GOSTOP project (smart specialization strategy) where we test the coatings for the partner Hidria.

Partners at the University of Bartin (Turkey) evaluated our TiAlSiN coating for the protection of cutting inserts for the milling of the Inconel 718 superalloy. In combination with the cryogenic treatment the tool lifetime was double its initial value. From a more basic point of view, our partners from the Vinča nuclear sciences institute (Serbia) studied the oxidation mechanisms of CrVN-based multilayer coatings; the oxidation was induced by the irradiation of nanosecond laser pulses. In the scope of the collaboration with the Institute of Metals and Technologies (Ljubljana) and the Faculty of Mechanical Engineering of the University of Ljubljana we published our results of wetting studies and friction control on nanostrucuted samples covered by super-hydrophobic silica nanoparticles.

In addition to the above-mentioned collaboration with foreign research institutions, the department's researchers work as guest scientists abroad. Our coworker Dr Aljaž Drnovšek spent two years as a postdoc at the Montanuniversität Leoben (Austria), and additionally worked as a guest at the University of Southampton (Great Britain) and the University of California, Berkley (USA). In the scope of that project he measured the high-temperature mechanical properties of CrAlN and CrAlSiN coatings, which among others includes measurements of nanohardness and toughness in the range from room temperature up to 700 °C. Despite the formal conclusion of the project, the collaboration is being continued.



At the end of 2017 we installed a new coating-deposition unit that applies cathodic arc evaporation. In industry Asst. Prof. Miha Čekada



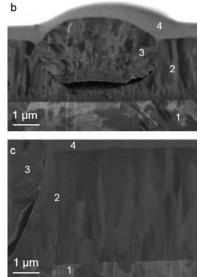


Figure 1: Cross-section of three TiN coatings deposited by different techniques: (a) evaporation by thermionic arc, (b) magnetron sputtering, (c) cathodic arc evaporation. Presented in the figures: substrate (1), undisturbed coating (2), growth defect (3) and protective layer for imaging (4). The images were acquired with the focused-ion-beam (FIB) technique.

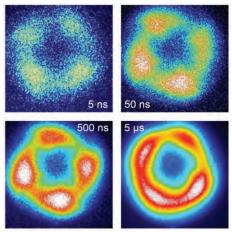


Figure 2: Magnetron plasma recorded with a highspeed camera at different exposure times

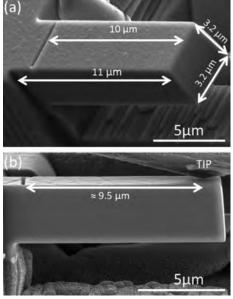


Figure 3: A microcantilever was constructed using a microscope with a focused ion beam, then it was broken in controlled conditions at elevated temperatures. Using sample geometry and braking forces we were able to determine the coating fracture toughness in dependence of the temperature.

# INTERNATIONAL PROJECTS

- H2020-EUROfusion-Plasma Facing Components-1-IPH-FU, EUROFUSION Dr. Matjaž Panjan European Commission
- H2020 EUROfusion Medium Size Tokamak Campaigns-MST1-FU Dr. Matjaž Panjan
- European Commission
- High-Temperature Tribological Behavior of Novel Hard Nanocomposite Nitride Coatings Dr. Peter Panjan Slovenian Research Agency

In order to deposit high-quality thin films it is important to have a good understanding of the plasma, such as ion density and ion energy. In this year we installed two important pieces of equipment, dedicated to plasma characterization: a high-speed camera and a mass spectrometer. The high-speed camera is predominantly used for studying the plasma dynamics, the inhomogeneities in plasma and for the observation of discharges and microparticles that appear in the plasma. The mass spectrometer with the ability to measure the ion energy is dedicated to the characterization of several types of low-pressure plasma that are used for the deposition of thin films.

Chemically speaking, our main research topic is transition-metal nitrides, both from the aspect of coating deposition as well as analyses of their properties. In addition, we are also active in the deposition and analytics of other materials, in most cases following the initiative of other research groups who do not have appropriate equipment for a particular segment of their research. In this way we collaborate with several other departments in our institute, and also with other institutions such as the Faculty of Electrical Engineering at the University of Ljubljana, Faculty of Mechanical Engineering of the University of Maribor and Vinča nuclear sciences institute. With the latter group we have continued the research of hematite nanoparticle magnetic properties. The department is also active in fusion research, being part of the Eurofusion project. In collaboration with the Max-Planck-Institut für Plasmaphysik from Garching (Germany) we investigate the damage to the tungsten plates that encircle the tokamak divertor; this damage is a consequence of plasma discharges during the reactor's operation.

Many companies get in touch with our department when there are some issues in production, if related to surfaces or thin films. It may be a question requiring advanced analytics or consulting related to solving a problem. In this year these analyses were made for the following Slovenian companies: Cetis, Hella Saturnus, Iskra mehanizmi, Kovinos, Marovt, Mines IB, Phos, SIQ Slovenia and Teroxal.

# Some outstanding publications in the past year

 P. Panjan, A. Drnovšek, J. Kovač, Tribological aspects related to the morphology of PVD hard coatings, *Surface & coatings technology*, 343 (2018), 138–147

# RESEARCH PROGRAM

1. Thin film structures and plasma surface engineering Asst. Prof. Miha Čekada

# R & D GRANTS AND CONTRACTS

- 1. Antibacterial Nanostructured Surfaces for Biological Applications Asst. Prof. Miha Čekada
- Understanding plasma processes and thin film growth in High Power Impulse Magnetron Sputtering Dr. Matjaž Panjan
- Building blocks, tools and systems for the Factories of the Future GOSTOP Asst. Prof. Mik Čekada
   Mikieta of Education Science and Spect

Ministry of Education, Science and Sport

# VISITORS FROM ABROAD

- Jelena Petruša, University of Zagreb, Zagreb, Croatia, 1. 1. 20. 7. 2018 1.
- Aleksandar Miletić, Dragan Kukuruzović, University of Novi Sad, Novi Sad, Serbia, 2 13.-15.6.2018
- 3. Marin Tadić, Vinča nuclear institute, Belgrade, Serbia, 1.-8. 8. 2018

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- 2 Dr. Peter Panjan
- Dr. Matjaž Panjan
- Postdoctoral associates 4. Dr. Aljaž Drnovšek
- Postgraduates
- Nastja Mahne, B. Sc.

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- Dragan Kukuruzović, University of Novi Sad, Novi Sad, Serbia, 24.-28. 9. 2018 5. 6.
- Marin Tadić, Vinča nuclear institute, Belgrade, Serbia, 17.-21. 12. 2018

Technical officers Uroš Stele, B. Sc Technical and administrative staff Jožko Fišer 8 Damjan Matelič 9. Andrej Mohar

10. Tomaž Sirnik

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- 6. Suzana Petrović, Biljana Gaković, Peter Panjan, Janez Kovač, Vladimir Lazović, C. Ristoscu, I. Negut, Ion N. Mihailescu, "Oxidation behaviour of composite CrN/(Cr,V)N coatings with different contents of vanadium induced by UV nanosecond laser pulses", Optical and quantum electronics, 2018, 50, 5, 208.
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# DEPARTMENT OF SURFACE ENGINEERING AND OPTOELECTRONICS F-4

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

The surface engineering of solid materials is often accomplished by the treatment of materials and products with non-equilibrium gaseous plasma. Such plasma is sustained by various electrical discharges in a range of powers up to about 10 kW. Suitable chambers of different dimensions have been developed and thoroughly verified by members of our research team. The plasma parameters depend on the applied power and coupling of the power supplies, pressure, gas flow through the discharge chamber and the properties of the materials facing Head: plasma. Although plasma parameters can be roughly estimated using our expertize, the exact values cannot **Prof. Miran Mozetič** be predicted; therefore, they should be measured. Numerous techniques for plasma characterization have been introduced worldwide, but none is capable of providing all the parameters; therefore, a combination of different techniques is necessary for thorough plasma characterization. A comprehensive description of available techniques for plasma diagnostics has been published as a monograph chapter [1].

Gaseous plasma is a source of charged particles, neutral reactive species and radiation. The radiaton appears in a broad range of wavelengths. Particularly important is radiation in the ultraviolet (UV) range, from about 200 to 350 nm. This radiation is often absorbed in the surface film of solid materials, where it causes modifications of the material's structure. The penetration depth of UV photons depends on the wavelength and the type of material. For organic materials it is roughly of the order of a micrometre. Radiation is particularly suitable for crosslinking the surface film of polymers. UV radiation appears during the relaxation of highly excited states of both charged and neutral gaseous species, but in weakly ionized plasma suitable for surface engineering radiation from neutral species prevails. Radiation arising from the relaxation of atoms is usually discrete, so the integral intensity is not very large. More efficient sources are excited molecules, which radiate either in bands or continua. Although the integral UV radiation from molecules is often much stronger than from atoms, it is rarely used due to a natural obstacle: molecules tend to dissociate to parent atoms more extensively than they are excited because the excitation energy of UV-radiating states is usually larger than the dissociation energy. As a result, the majority of available discharge power is used for dissociation rather than UV radiation. This effect suppresses the efficiency of plasma UV sources. Our research team, however, managed to develop a powerful source of the UV radiation based on the excitation of molecular states of SO, radicals. Energy efficacy of such UV sources is superior to other types of large-volume UV sources and is thus particularly suitable for the cross-linking

of polymers that cannot withstand elevated temperatures. An appropriate patent application has been filed in 2016 and the patent was granted by the EU office in Munich in December 2018 [2]. The superior property of our innovative device is revealed by a comparison of plasma spectra with a commonly used commercial low-pressure mercury lamp. The spectra shown in Figure 1 were measured with the same spectrometer using the same integration time. Not only is our innovative plasma source much more efficient, but it also lacks radiation in the visible range, which causes extensive heating of the treated materials.

The research team also invented other plasma solutions of commercial interest and filled the appropriate patent applications. The application "Carbon nanostructured materials and methods for forming carbon nanostructured materials" discloses an original method for depositing carbon nanowalls using carbon dioxide as the precursor. The method is scalable to industrial-size substrates and enables a deposition rate of about 100 nm/s, which is one of the largest rates ever reported for the deposition



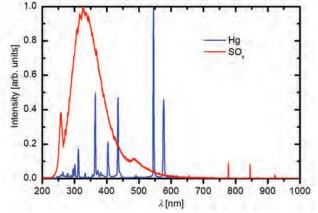


Figure 1: Spectra from a commercial Hg lamp (blue curve) and our patented source (red curve).

of carbon nanostructures using non-equilibrium gaseous plasma. The patent application "Method for treatment medical devices made from nickel - titanium (NiTi) alloys" discloses a plasma technique that provides excellent biocompatibility. Not only is the activation of blood platelets supressed significantly, as compared to the known techniques for surface finishing of this alloy, but the methods of invention enable rapid edothellization as well.

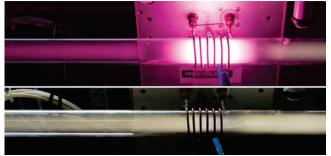


Figure 2: Ammonia plasma in E-mode (lower photo) and H-mode (upper photo).

The technique is therefore suitable for the modification of commercial vascular stents made from this alloy. The third patent application filed in 2018 reveals a technique for the purification of biologically contaminated water. The application "Method for deactivation of a virus in water" protects our innovative technology, which takes advantage of the differences in the surface free-energy between water and organic materials, such as a virus. Viruses accumulate on the surface of bubbles containing water vapour, and the vapour is preferentially heated by gaseous plasma to high temperatures to produce a sterilization effect.

Low-pressure ammonia plasma is used for the surface modification of various materials. Reactive gaseous species produced in ammonia plasma can be used for surface etching and thus removing undesired oxides or deposits, functionalization of surfaces with N-containing functional groups or for synthesizing various nitrides. Even though

ammonia plasma is often used for the surface treatment and despite evident usefulness, the characteristics of ammonia plasma have not been studied thoroughly yet and no systematic measurements of the properties of low-pressure ammonia inductively coupled plasma (ICP) have been reported in the scientific literature. Lowpressure ammonia ICP plasma operates in two regimes: the so-called E and H modes. Images of both modes are shown in Figure 2. In the E-mode, plasma is partially dissociated and the main reactive species are NH and NH, radicals. Such plasma is particularly suitable for the treatment of delicate materials, for example, functionalization of polymer materials with nitrogen-containing groups including amino (-NH<sub>2</sub>) groups. In H-mode, ammonia molecules are almost fully dissociated. In this case, the optical spectrum reveals only H and N atoms and some radiation arising from NH radicals, as well as N<sub>2</sub> molecular bands indicating partial association of N atoms to nitrogen molecules. Plasma in H-mode is therefore more suitable for etching or nitriding than functionalization with amino groups. Our detailed characterization of ammonia ICP plasma at different pressures and discharge powers showed hysteresis during transitions between E and H modes. Figure 3 shows the hysteresis in intensity arising from the excited NH radical. We systematically measured the behaviour of different nitrogen-containing reactive gaseous species in relation to discharge power and pressure. We have also found that the etching rate of the PET polymer in E-mode ammonia plasma is approximately a hundred times lower than in the H-mode under otherwise comparable discharge parameters. A detailed description of this phenomenon was published in an extensive article [3].

Neutral gaseous radicals are not stable, but are lost by different gas-phase and surface reactions. The loss rates influence plasma properties significantly. Therefore, the knowledge of how extensively atoms are lost on the surfaces of materials facing plasma is equally important as the knowledge of how they are produced in gaseous discharge. In order to estimate the atom density, one should know the atom-loss coefficient for different atoms and for various materials. Surface-loss rate is often expressed in terms of the recombination coefficient.

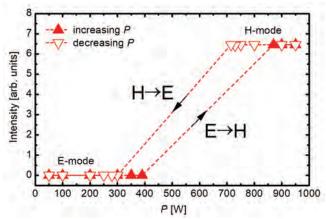


Figure 3: Hysteresis of the NH optical emission peak intensity at transitions between the E and H modes.

Coefficients for some materials, such as metals, metal oxides, ceramics and glasses, have been measured by different authors using different techniques for decades and are easily found in the literature. The coefficients for polymers, however, have been measured rarely and results obtained by different authors vary significantly. Using our original technique, we systematically measured loss rates of hydrogen and oxygen atoms on the surface of three technologically important polymers: polyethylene terephthalate (PET), polystyrene (PS) and polytretrafluoroethylene (PTFE, often known as Teflon) at different fluxes of either type of atoms onto the polymer samples. We confirmed the hypothesis that the coefficient does not depend much on the atom flux since the surface quickly saturates with adsorbed atoms. The largest coefficient for hydrogen atoms was determined for PET and was approximately 0.0023 and the lowest was 0.0008 for PTFE (Teflon). The PTFE also exhibited the lowest coefficient for the heterogeneous surface recombination of oxygen atoms, which was approximately 0.001. The results are useful for numerous users of plasma technologies for tailoring surface properties of polymer materials. The corresponding paper was published as [4].

Although gaseous plasma has been used for surface functionalization of polymers on an industrial scale for decades, the scientific background on the initial stages of polymer functionalisation upon interaction with neutral oxygen atoms remained unknown, due to the lack of appropriate experimental setups. We managed to reveal the interaction kinetics by dosing O atoms in a highly precise manner. The preparation chamber of our

XPS instrument was equipped with a source of O atoms that enabled an adjustable density of atoms in the ground state in a broad range from 3×10<sup>16</sup> to 3×10<sup>20</sup> m<sup>-3</sup>. Such a huge range enabled the exposure of a polystyrene sample to O atoms of almost arbitrary fluences. Vacuum conditions were not broken between the exposure in the XPS pre-chamber and the characterization in the XPS main chamber; therefore, measurements were very reliable. We found that the initial reaction was breakage of the phenyl ring, because the intensity of the characteristic XPS shakeup peak dropped by more than a factor of two, even for a fluence as low as 2×10<sup>21</sup> m<sup>-2</sup>. Simultaneously, the hydroxyl functional group appeared on the sample surface. Other functional groups appeared at larger fluences. For example, the highly polar O-C=O functional group became measurable at fluences above 10<sup>22</sup> m<sup>-2</sup>. While the surface concentration of the hydroxyl group saturated at a fluence of about 10<sup>23</sup> m<sup>-2</sup>, other groups kept increasing with the increasing fluence of oxygen atoms. The characteristic shakeup peak was not influenced much after the sample received a fluence of approximately 2×10<sup>21</sup> m<sup>-2</sup> indicating that functionalization was limited to a very thin surface film, definitely thinner than the mean free path of the photoelectrons [5]. The behaviour of all the functional groups versus the O-atom fluence is shown in Figure 4.

Weakly ionized plasma, rich in neutral radicals, is suitable for surface functionalization, but almost useless when charged particles are the key reactants. This is the case when plasma is used for sputtering solid materials and thus the transfer of material from a target to a substrate. In collaboration with the Institute of Solid State Physics from Vienna University of Technology, Austria, we employed a moderately ionized gaseous plasma for the deposition of thin metal films. The films were then oxidized in our labs by treating them with a rather mild oxygen plasma. The original hypothesis was that the oxygen plasma treatment of zirconia alloys leads to the preferential formation of tetragonal zirconium dioxide (ZrO<sub>2</sub>), which exhibits very good photocatalytic activity. We investigated the range of parameters where the stabilization of tetragonal zirconium dioxide was possible with alternative dopants, like aluminum or copper. Thin metallic films were produced with a dual-cathode magnetron-sputtering device using energetic argon ions. The deposited films resembled ZrAl and ZrCu alloys. After synthesizing they were further treated with oxygen plasma and then thoroughly characterized. Depth profiles were recorded by Auger electron spectroscopy (AES) to follow the film's composition and the progress of the oxidation. For the crystallographic analysis, X-ray diffraction (XRD) was employed, while the evolution of the surface morphology was determined by atomic force microscopy (AFM). Within a limited range of deposition and oxidation parameters, we managed to obtain tetragonal zirconia when copper was used for the stabilization. In the case of aluminum, no formation of the tetragonal ZrO<sub>2</sub> phase was observed over a broad range of parameters. The doping of Zr with Cu and subsequent treatment with oxygen plasma was therefore found to be a promising method for the stabilization of tetragonal zirconia. We managed to obtain the desired properties with a brief oxygen-plasma treatment of the order of seconds, and the method could also be scaled up using larger samples and treatment chambers [6]. This work can be considered as a proof of concept, and further work will be done with respect to the optimization of the dopant content and plasma treatment parameters.

Using surface-sensitive techniques such as time-of-flight secondary-ion mass spectroscopy (ToF-SIMS), X-ray photoelectron spectroscopy (XPS) and AFM we studied the adsorption of two corrosion inhibitors, propargyl

alcohol (PA) and cinnamaldehyde (CIN) on a steel surface. These compounds are known to be effective corrosion inhibitors for lower-grade steel materials in acidising oilfield applications. We managed to confirm the adsorption of cinnamaldehyde and propargyl alcohol molecules on a steel surface due to the low detection limit and selectivity of the ToF-SIMS method, even for very thin layers of thickness in the nm range. In the

The desorption kinetics of selected corrosion inhibitors has been revealed for the first time anywhere in the world.

ToF-SIMS analysis of the CIN corrosion inhibitor, a signal related to the CIN molecule was identified at 131.04 Da, corresponding to  $C_0H_2O^+$  ions. The adsorption of PA molecules was also confirmed by a signal at 55.02 Da

## The formation of different functional groups on a polymer surface upon treatment with O atoms has been revealed.

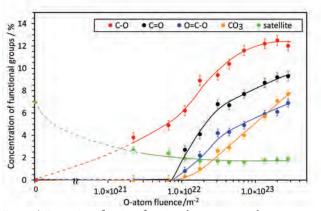


Figure 4: Formation of various functional groups on a polystyrene surface versus fluence of 0 atoms in the ground state.

 $(C_3H_3O^*)$  related to the PA molecule in the positive part of the ion spectrum. The possibility of spatially resolved ToF-SIMS analyses with a high mass resolution allowed us to follow the lateral distribution of the adsorbed corrosion inhibitors. We managed to identify the non-homogenous distribution of CIN molecules on a steel surface, as revealed by Figure 5. A more homogenous distribution was observed for PA molecules on the steel surface, but

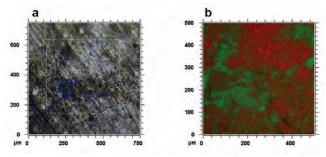


Figure 5: Optical (a) and ToF-SIMS molecular specific image (b) of the spatial distribution of the corrosion inhibitor cinnamaldehyde adsorbed on the C15 steel over an area of  $500 \times 500 \,\mu m^2$ .

some PA agglomerates were detected. For the first time anywhere in the world we showed that by using the SIMS method it was possible to study the temperature stability of corrosion inhibitors by annealing the samples and performing an *in-situ* ToF-SIMS analysis [7]. We estimated the desorption temperature for the CIN corrosion inhibitor to be  $150 \pm 10$  °C, from which the desorption energy for the CIN layer on the C15 steel was calculated to be  $122 \pm 5$  kJ/mol. For the PA corrosion inhibitor, desorption from C15 steel occurs over a wider temperature range between 100 °C and 300 °C, which allowed us to estimate the desorption energy for the PA corrosion inhibitor to be in the range of 107–167 kJ/mol.

In collaboration with the Department of Nanostructured Materials we invented a novel approach to synthesize electrically conductive ceramics reinforced by cellulose nanofibers. This material exhibits a rather high electrical conductivity and dielectric permittivity. Some rather hydropho-

bic nano-cellulose was introduced into alumina and yttria-stabilized zirconia at concentrations between 0.5 and 3 wt.%. A sintering procedure was performed using the spark-plasma technique. XPS characterization revealed the transformation of the cellulose fibrils into two-dimensional graphitic sheets upon heating during sintering. The sheets represented the key to remarkable electronic and dielectric properties. Thermal conductivity was actually decoupled from electron conductivity. We envisage that our results can pave the way to better composite materials for telecommunication and energy applications. The results of our research on these composite ceramics were published as [8].

Our research team has been involved in fusion-oriented research since 2005. A major contribution of our team is studying details about the interaction of hot hydrogen plasma with solid materials. The results of our research are useful for a better understanding of the plasma behaviour in current large and medium-sized fusion plasma reactors, as well as for giving directions about the construction details of future fusion reactors, including the largest international experimental thermofusion reactor (ITER), which is built in France. The vacuum chamber of the ITER plasma reactor weights 8000 tonnes and is made of special grade stainless steel. Tritium retention may represent a serious safety threat. Among the activities which could contribute to a more accurate prediction of the tritium retention was also our study of hydrogen permeation through the austenitic steel membranes AISI 316 LN ITER grade. Our measurements were carried out at different temperatures between 100 and 400 °C and in the pressure range between 50 and 1000 mbar. All membranes were only covered by native oxides, which were evidently modified by baking in vacuum conditions at 160 °C. This fact may be assumed relevant for the ITER operation, as similar conditions regarding the residual atmosphere could be readily met during every vacuum bake-out cycle [9].

Another important technological challenge is the long-term maintenance of low pressure in thermal insulat-



Figure 6: Prof Janez Kovač opened the meeting organized by Strategic Partnership "Factories of Future".

ing vacuum devices. Even in completely tight metal envelopes, gas accumulation, due to the outgassing of applied materials, represents the main problem. Among the gases that are not desorbed completely during pre-processing and which are dissolved in constructional metals, hydrogen is the most harmful. Fortunately, it is also the only gas that might permeate through the metallic envelopes. If we could effectively pump hydrogen the problem would be solved. So far, the selective pumping of hydrogen has not been realized. A heated metal membrane made of martensitic steel Eurofer was fixed to an extended part of a tight ultra-high vacuum (UHV) chamber. The initial hydrogen pressure was set in a broad range from 1.5 bar to 1×10<sup>-3</sup> mbar at temperatures from 100 to 400 °C. The observed hydrogen permeation flow was expressed in the terms of the specific pumping speed, which is defined as the volume flow of hydrogen per unit surface area. At a pressure of 1 mbar and a temperature of 400 °C the permeation was about 1.6×10<sup>-6</sup> L s<sup>-1</sup>cm<sup>-2</sup>. This is about the value needed in numerous applications so the membrane may be used as an innovative pump in specific applications. At lower pressures, this attractive pump performance was overwhelmed by the background outgassing of carbon dioxide and monoxide. At temperatures lower than 200 °C, the outgassing rate of carbon oxides was not detectable and the pumping continued into the 10<sup>-4</sup> mbar pressure range.

Researchers have been active in the preparation of the Slovenian Smart Specialisation Strategy (S4), which is the key strategic document for the modernization of the Slovenian economy and the development of specific sectors that have been indicated as comparative advantages of our country. Smart specialisation is a platform for concentrating development investments in areas where Slovenia has the critical mass of knowledge, capacities and competences and where there is innovation potential for placing Slovenia within global markets and thus enhancing its recognisability. Plasma technologies have been recognized as one of six key emerging technologies and a member of our research team has been assigned the leader of this horizontal activity. Furthermore, the head of our research team has been assigned as Board Member of the Strategic Research and Innovation Partnership "Factories of Future". The action plan has been prepared and it includes R&D projects that will enable the introduction of plasma technologies into various sectors from the electronics industry to agriculture. Several meetings have been organized, with the aim of networking between the academic sector and industry. Numerous scientists and business people, renowned worldwide in the niche of plasma technologies, attended the meetings. Among the meetings, we organized a conference on vacuum science and technology, which was chaired by a group member, Prof. Janez Kovač (Figure 6).

# Some outstanding publications in the past three years

- Mozetič, Miran, Vesel, Alenka, Primc, Gregor, Zaplotnik, Rok. Introduction to plasma and plasma diagnostics in Non-thermal plasma technology for polymeric materials: applications in composites, nanostructured materials, and biomedical fields. Amsterdam: Elsevier, 2019, 23-65.
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- 2. Marián Lehocký, Petr Stloukal, Vladimír Sedlarik, Petr Humpolíček, Alenka Vesel, Miran Mozetič, Rok Zaplotnik, Gregor Primc, Device and method for producing UV radiation, EP3168860 (B1), European Patent Office, 19. 12. 2018.

# INTERNATIONAL PROJECTS

 COST CA15114; Anti-Microbal Coating Innovations to prevent Infectious Diseases (AMICI)
 Prof. Uroš Cvelbar

- COST TD1305; Improved Protection of Medical Devices Against Infection (IPROMEDAI) Dr. Martina Modic Cost Office
- H2020 PEGASUS; Plasma Enabled and Graphene Allowed Synthesis of Unique nano Structures
  - Prof. Uroš Cvelbar
- European Commission
- 4. H2020-EUROfusion-Plasma Facing Components-1-IPH-FU, EUROFUSION

Asst. Prof. Rok Zaplotnik European Commission

- 5. H2020 EUROfusion Education-ED-FU Prof. Miran Mozetič
  - European Commission
- H2020 EUROfusion Medium Size Tokamak Campaigns-MST1-FU Asst. Prof. Rok Zaplotnik European Commission
- Making Luminescent C-dots and GQDs Based on Atmospheric Pressure Microplasma-Liquid Interaction Prof. Uroš Cvelbar
- Slovenian Research Agency

Cost Office



- Quantitative Depth Profiling of Ultra-Thin Films Prof. Janez Kovač Slovenian Research Agency
- Catalytic Activity of Nanomaterials for Elimination of Sulfur Prof. Uroš Cvelbar
- Slovenian Research Agency
- 10. Determination of Neutral-Atom Densities in Large Plasma Reactors Prof. Miran Mozetič
- Slovenian Research Agency 11. Plasma Assisted-Deposition of An
- Plasma Assisted-Deposition of Antibacterial Coatings and their Testing Dr. Martina Modic Slovenian Research Agency
- Plasma-Assisted Design of Multifunctional Carbon Nanowalls Bio-Sensor Prof. Uroš Cvelbar
- Slovenian Research Agency 13. Innovative Coatings for Bare Metallic Vascular Stents for Reduction of Restenosis and Acceleration of Natural Endothelization Prof. Miran Mozetič
  - Slovenian Research Agency
- Transport and Pield Emission Properties of Low-Dimensional Molybdenum and Tungsten Based Nanomaterials Dr. Vincenc Nemanič
  - Slovenian Research Agency
- DST Treasurer of ECS Division Dielectric Science and Technology DST, eElection ECS Prof. Uroš Cvelbar
- Slovenian Research Agency 16. Catalytic Probes for Characterization of Hydrogen Plasma
- Asst. Prof. Gregor Primc
- Slovenian Research Agency 17. Control of Chemical Composition of Thin Films by High Resolution Mass Spectrometry of Secondary Ions
- Prof. Janez Kovač
- Slovenian Research Agency
- 18. Advanced Catalysts based on Multilayered Vertically Oriented Graphene Nanostructures Prof. Alenka Vesel
- Slovenian Research Agency 19. Consequences of electron emission from hot plasma-facing components in nuclear fusion reactors
- Prof. Miran Mozetič Slovenian Research Agency

# 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. Nanoscale engineering of the contract interfaces for green lubrication technology Prof. Janez Kovač
- Multifunctional electrospunned nanofibers development and dynamic interaction studies with pathogen bacteria Prof. Miran Mozetič
- Understanding plasma processes and thin film growth in High Power Impulse Magnetron Sputtering Prof. Uroš Cvelbar
- Plasma-assisted wound treatment and topical introduction of molecules Prof. Uroš Cvelbar
- 5. Novel higly sensitive and fast water qulity monitoring sensors Prof. Uroš Cvelbar

# VISITORS FROM ABROAD

- Dr. Marian Lehocky, Tomas Bata University, Zlin, Czech Republic, 16–17 January 2018
   Dr. Danijela Vujošević, Institute for Public Health of Montenegro, Podgorica,
- Montenégro, 18–21 January 2018
- 3. Prof. Hiroki Kondo, Nagoya University, Nagoya, Japan, 16–20 January 2018
- Prof. Jiang Yong Wang, Shantou University, Shantou, China, 30 January-5 February 2018
   Dr. Johannes Gruenwald, Gruenwald Laboratories GmbH, Taxenbach, Austria, 21–23
- Dr. Johannes Gruenwald, Gruenwald Laboratories GmbH, Taxenbach, Austria, 21-March 2018
- 6. Dr. Endre Szili, University of South Australia, Adelaide, Australia, 22–27 March 2018
- Dr. James Walsh, University of Liverpool, Liverpool, United Kingdom, 16–27 April 2018
   Dr. Davor Peruško, Vinča Institute of Nuclear Science, Belgrade, Serbia, 13–19 May 2018
- D. Davor rerusko, vinca institute of Nuclear Science, Belgrade, Serbia, 15–19 May 2018
   Dr. Suzana Petrović, Vinča Institute of Nuclear Science, Belgrade, Serbia, 13–19 May 2018

- Advanced surface finishing technologies for antibacterial properties of patient specific 3D printed implantable materials Asst. Prof. Ita Iunkar
- New generation of superior creep resistant steels with nanoparticles modified microstructure Prof. Uroš Cvelbar
- Development of new, environment-friendly approaches for plant and human virus inactivation in waters
- Asst. Prof. Gregor Primc 9. Advanced hydrodesulphurisation with catalyst nanomaterials
- Auvanceu nyurouesuipirurisation with catalyst nanomaterial Prof. Uroš Cvelbar
- 10. Advanced hemocompatible surfaces of vascular stents Asst. Prof. Ita Junkar
- 11. Evaluation of the range of plasma parameters suitable for nanostructuring of polymers on industrial scale
- Prof. Miran Mozetič12. Selective plasma oxidation of FeCrAl alloys for extended-lifetime of glow plugs for diesel engines

## Prof. Janez Kovač

- Innovative configuration of inductively coupled gaseous plasma sources for up-scaling to industrial-size reactors
- Prof. Miran Mozetič 14. Food for future - F4F
- Prof. Alenka Vesel
- Ministry of Education, Science and Sport
- 15. Potential of biomass for development of advanced materials and bio-based products Asst. Prof. Ita Junkar
- Ministry of Education, Science and Sport 16. Building blocks, tools and systems for the Factories of the Future – GOSTOP Prof. Miran Mozetič
- Ministry of Education, Science and Sport
- Development of nanostructured biosensors for diagnosis/treatment of cancer and surfaces with antibacterial Dr. Metka Benčina
- Ministry of Education, Science and Sport
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Miran Mozetič
- Ministry of Economic Development and Technology 19. Novel type of antibacterial coatings on textile materials and plastics with controllable
- Nover type of antibacterial coatings on textile materials and plastics with controllable release of antibacterial agent Prof. Uroš Cvelbar
- Ministry of Education, Science and Sport
- Preparation and Analysis of Samples for Customer Prof. Uroš Cvelbar
  - Tomas Bata University in Zlin
- Income from Coowners of Invention for Reimbursement of Costs for IP Protection in the Case of EVT140\_Mozetič\_Carbon Nanowall Prof. Miran Mozetič Nagoya University

# NEW CONTRACTS

- 1. Ecologically benign technology for joining polymeric products Asst. Prof. Gregor Primc
- Simtrona d. o. o.
- Innovative configuration of inductively coupled gaseous plasma sources for up-scaling to industrial-size reactors Prof. Miran Mozetič
- Vacutech Vakuumske Tehnologije in Sistemi d. o. o.
- Regulation of mutual relations between the Company and JSI in joint research and development ("KET4CleanProduction")

Asst. Prof. Ita Junkar Brinox Inženiring d. o. o.

- 10. Dr. Robert Olejnik, Tomas Bata University, Zlin, Czech Republic 13–19 May 2018
- Dr. Robert Olejnik, Tomas Bata University, Zlin, Czech Republic, 21–26 May 2018
   Prof. Dr. Nandakumar Kalarikkal, Mahatma Gandhi University, Kottayam, India,
- Prof. Dr. Nahdakumar Kalarikkal, F 3–7 June 201
- June 201
   Prof. Paul Paulsen, University of Vienna, Vienna, Austria, 5 July 2018
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- Dr. James walsh, University of Liverpool, Liverpool, United Kingdom, 5 July
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- 16. Prof. Zdenko Machala, Comenius University, Nagoya, Japan, 4–7 July 2018
   16. Prof. Zdenko Machala, Comenius University, Bratislava, Slovakia, 5–6 July 2018
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   Dr. Petr Slobodian, Tomas Bata University, Zlin, Czech Republic, 4–6 July 2018
- 18. Prof. Masaru Hori, Nagoya University, Nagoya, Japan, 4-7 July 2018

- 19. Prof. Kursat Kazmanli, Prof. Dr. Mustafa Kamil Ürgen, Dr. Cagatay Yelkarasi, Istanbul Technical University, Istanbul, Turkey, 3-7 July 2018 20. Dr. Danijela Vujošević, Institute for Public Health of Montenegro, Podgorica,
- Montenegro, 13-16 September 2018

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21. Dr. Cagatay Yelkarasi, Istanbul Technical University, Istanbul, Turkey, 6-17 December 2018

#### Postgraduates

- 15. Nataša Hojnik, B. Sc. 16. Matej Holc, B. Sc. 17. Martin Košiček, B. Sc. Dane Lojen, B. Sc.
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- 25. Maja Šukarov, B. Sc.
- 26. Janez Trtnik
- 12. Nikola Škoro, Nevena Puač, Suzana Živković, Dijana Krstić-Milošević, Uroš Cvelbar, Gordana Malović, Zoran Lj. Petrović, "Destruction of chemical warfare surrogates using a portable atmospheric pressure plasma jet", The European physical journal. D, Atomic, molecular and optical physics, 2018, 72, 2.
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- 19. Matej Holc, Rok Zaplotnik, Miran Mozetič, Alenka Vesel, "Surface modification and aging of polyacrylonitrile butadiene styrene polymer induced by treatment in RF oxygen plasma", IEEE transactions on plasma science, 2018, 46, 10, 3669-3676.
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# MONOGRAPH

- Tina Mavrič, Metka Benčina, Roghayeh Imani, Ita Junkar, Matjaž Valant, Veronika Kralj-Iglič, Aleš Iglič, "Electrochemical biosensor based on TiO<sub>2</sub> nanomaterials for cancer diagnostics", In: Aleš Iglič (ed.), Michael Rappolt (ed.), Ana J. García-Sáez (ed.), (Advances in biomembranes and lipid self-assembly **27**) 2018,, 63-105.
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## MENTORING

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# DEPARTMENT OF SOLID STATE PHYSICS

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

The experimental techniques used are:

- One (1D) and two (2D) dimensional nuclear magnetic resonance (NMR) and relaxation, as well as quadrupole (NQR) resonance and relaxation,
- Multi-frequency NMR in superconducting magnets of 2T, 6T and 9T, as well as the dispersion of the spin-lattice relaxation time t, via field cycling,
- Nuclear double resonance and quadrupole double resonance such as <sup>17</sup>O-H and <sup>14</sup>N-H,
- Fast field cycling NMR relaxometry,
- Frequency-dependent electron paramagnetic resonance (EPR) and 1D and 2D pulsed EPR and relaxation,
- MR imaging and micro-imaging,
- Measurement of the electronic transport properties,
- Magnetic measurements,
- Fluorescence confocal microscopy and microspectroscopy,
- Linear and non-linear dielectric spectroscopy in the range 10<sup>-2</sup> Hz to 10<sup>9</sup> Hz,
- Electron microscopy and scanning-tunnelling microscopy,
- Atomic force microscopy and force spectroscopy,
- Dynamic specific-heat measurements,
- Low-temperature scanning-tunnelling microscopy and single-atom manipulation,
- Atomic Force Microscopy,
- Manipulation of particles with laser tweezers,
- Super-resolution STED microscopy,
- Laser cooling and manipulation of Cs atoms.

The research program of the Department of Solid State Physics at the Jožef Stefan Institute is performed in close collaboration with Department of Physics at the Faculty of Mathematics and Physics of the University of Ljubljana, Institute of Mathematics, Physics and Mechanics and the Jožef Stefan International Postgraduate School. In 2018, the research was performed within three research programs:

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

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

The research of the programme 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 these investigations was to discover the basic laws of physics governing the behaviour of the investigated systems. The acquired knowledge provides the key to the understanding of the microscopic and



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Prof. Igor Muševič

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

In our research we used the following experimental techniques:

- Nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR) and nuclear quadrupole resonance (NQR),
- Nuclear double resonance <sup>17</sup>O-H and <sup>14</sup>N-H,
- Fast field cycling NMR relaxometry,
- Linear and non-linear dielectric spectroscopy in the range 10<sup>-2</sup> Hz to 10<sup>9</sup> Hz,
- Frequency-dependent ac calorimetry,
- Measurement of electrical and thermal transport coefficients,
- Magnetic measurements,
- Methods of ultra-cold atoms.

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

In 2018, members of the programme group published 38 original scientific papers in international peer-reviewed scientific journals, two book chapters and obtained two US patents. Among these, one paper was published in Nature Physics (IF = 22.7), one in Adv. Mater. (IF = 22), one in Nano Letters (IF = 12.1), one in Sci. Adv. (IF = 11.5), one in J. Mater. Chem. (IF = 9.9), two in Phys. Rev. Lett. (IF = 8.8) and 15 papers in the journals with an IF between 3.0 and 5.0.

The investigations were focused to the following research fields:

#### 1. Quantum magnetism

Andrej Zorko, Peter Jeglič, Matej Pregelj, and Denis Arčon, in collaboration with partners from Switzerland, Germany, and Russia, studied the magnetic properties of the layered compound CuNCN with several experimental techniques, including NMR, NQR, and mu-SR. The investigation revealed a magnetically frozen and disordered magnetic ground state. The authors showed that regions of magnetically frozen and paramagnetic phases coexist on a microscopic level in this compound below the freezing temperature in a broad temperature range. The results were published in the paper A. Zorko *et al.* "Magnetic inhomogeneity in the copper pseudochalcogenide CuNCN",

The research group has presented the first experimental proof of the existence of "anyone" particles (the particles that are simultaneously fermions and bozons) and discovered new quantum magnetic states in solid-state materials. It has found new multiferroic materials, revealed complex magnetism of high-entropy alloys, developed fully printed thin-film capacitors and determined the physical-mechanical properties of liquid crystals and liquid-crystalline elastomers.

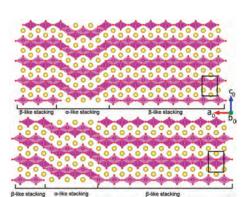


Figure 1: Incommensurate, compositionally modulated crystal structure of β-NaMnO<sub>π</sub>

Phys. Rev. B 97, 214432 (2018).

Andrej Zorko and Denis Arčon, in collaboration with partners from the United Kingdom, Greece and Germany, employed a combination of complementary experimental techniques, including heat-capacity measurements, NMR and elastic and inelastic neutron scattering to investigate the structural and magnetic properties of the geometrically frustrated antiferromagnet  $\beta$ -NaMnO<sub>2</sub>. The measurements disclosed the existence of novel structural degrees of freedom, which are incompatible with any commensurate order and are instead explained by an incommensurate compositionally modulated crystal structure. Such a structure leads to an incommensurate, that is, inhomogeneous, cooperative magnetism. The discovery was published in the paper F. Orlandi *et al.* "Incommensurate

atomic and magnetic modulations in the spin-frustrated  $\beta$ -NaMnO<sub>2</sub> triangular lattice", *Phys. Rev. Materials* 2, 074407 (2018).

Andrej Zorko, in collaboration with partners from Croatia, France and the USA, discovered the first crystal structures of oxo-bridged [Cr<sup>III</sup>Ta<sup>V</sup>] dinuclear complexes. The new structure complies with theoretical predictions based on DFT calculations. The compound was also magnetically characterized by the use of bulk SQUID magnetometry and a local-probe ESR technique. Also, these experimental results agree well with DFT-based expectations. The discovery was published in the paper L. Androš Dubraja *et al.* "First crystal structures of oxo-bridged [Cr<sup>III</sup>Ta<sup>V</sup>] dinuclear complexes: spectroscopic, magnetic and theoretical investigations of the Cr–O–Ta core", *New J. Chem.* **42**, 10912 (2018).

Matej Pregelj, Andrej Zorko and Denis Arčon, in collaboration with partners from Switzerland and Austria, discovered the coexistence of spinon and magnon excitations in the beta-TeVO<sub>4</sub> system. Their work is a rare demonstration of the coexistence of fractional and collective excitations in a system of weakly coupled, frustrated, zigzag spin chains. The team reproduced the experimental dispersion relations, derived from inelastic neutron scattering, using the linear-spin-wave-theory calculations and pre-calculated spinon dispersion. This allowed them to quantitatively determine the main exchange interactions and their anisotropies. The discovery was published in the paper M. Pregelj *et al.* "Coexisting spinons and magnons in the frustrated zigzag spin-1/2 chain compound  $\beta$ -TeVO<sub>4</sub>", *Phys. Rev. B* **98**, 094405 (2018).

Matej Pregelj, Nejc Janša and Denis Arčon, in collaboration with partners from Italy and Brazil, investigated spin fluctuations in a high-spin state of cobalt valence tautomer. A reversible transition from a low- to a high-spin state can be induced by temperature, pressure and light irradiation. The team investigated spin dynamics by nuclear-magnetic-resonance, muon-spin-relaxation and magnetization measurements. They found that at low temperatures (30 K) the high-spin state can be induced by light irradiation, which has a lifetime of several hours and occurs in the MHz frequency range. The discovery was published in the paper F. Caracciolo *et al.* "Spin fluctuations in the light-induced high-spin state of cobalt valence tautomers", *Phys. Rev. B* 98, 054416 (2018).

Nejc Janša, Andrej Zorko, Matjaž Gomilšek, Matej Pregelj and Martin Klanjšek, together with partners from Switzerland, experimentally demonstrated that a spin flip in the most promising Kitaev honeycomb magnet, in ruthenium trichloride, fractionalizes into a Majorana fermion and a pair of gauge fluxes, in line with the famous Kitaev prediction. Both types of fractional quasiparticles behave as neither pure fermions nor pure bosons, but rather as anyons. As they are both found to survive in a broad range of temperatures and magnetic fields, this discovery establishes ruthenium trichloride as a unique platform for future investigations of anyons. The work was published in the article N. Janša *et al.*, "Observation of two types of fractional excitation in the Kitaev honeycomb magnet", *Nature Physics* 14, 786 (2018).

Denis Arčon, Peter Jeglič and Tilen Knaflič discovered a Verwey-type charge ordering and electron localization transition in a compound that is composed of negatively charged dioxygen molecules. One of the very first attempts to understand the charge dynamics in mixed-valence systems dates back to 1939 when Evert Verwey, a Dutch chemist, observed a sudden jump in resistivity near -150°C in magnetite. A research team of scientists from Germany and Slovenia reported a Verwey-type transition in a completely different class of mixed-valence compounds, which is composed of negatively charged dioxygen molecular. The compound  $Cs_4O_6$  undergoes a phase transition from a state with indistinguishable molecular  $O_2^{x}$  entities to a state with well-defined superoxide  $O_2$  and peroxide  $O_2^{2^2}$  anions. The breakthrough of this study is the observation of such a charge ordering in a simple crystal structure where novel physical phenomena are expected to emerge from intertwining of the degrees of freedom pertinent to electronically active oxygen molecular units. The work was published in P. Adler *et al.*, "Verwey-type charge ordering transition in an open-shell p-electron compound", *Science advances* 4, eaap7581 (2018).

### 2. Magnetism of CeGdTbDyHo high-entropy alloy

We have investigated the magnetism of the CeGdTbDyHo high-entropy alloy, composed of rare-earth elements that mix ideally in a solid solution. This high-entropy alloy forms an almost undistorted hexagonal crystal lattice (Figure 5), which possesses an enormous chemical disorder. The structure is stabilized entropically by the mixing entropy term  $T\Delta S_{mix}$  in the Gibbs free energy.

By measuring the magnetic susceptibility, the magnetoresistance and the specific heat, we have determined the (H, T) magnetic phase diagram, which contains a helical antiferromagnetic state at elevated temperatures and a disordered ferromagnetic state at low temperatures (Figure 6).

Published in: S. Vrtnik, J. Lužnik, P. Koželj, A. Jelen, J. Luzar, Z. Jagličić, A. Meden, M. Feuerbacher, J. Dolinšek. Disordered ferromagnetic state in the Ce-Gd-Tb-Dy-Ho hexagonal high-entropy alloy. *Journal of Alloys and Compounds* 742 (2018), 877-886.

# 3. Study of nanostructured materials and materials with large caloric effects for solid-state cooling applications

Ferroelectric relaxors are an important class of materials that exhibit extraordinary ferroelectric, dielectric, piezoelectric, and electrocaloric properties. The physical reason behind these extraordinary properties of relaxors are the so-called polar nanoregions (PNRs). In this study we investigate the impact of PNRs on the polarization and electrocaloric properties by utilizing the dynamic pair distribution function (DPDF) technique. The DPDF indicates the distance between a specific atomic pair, while the peak height corresponds to the probability of finding such an

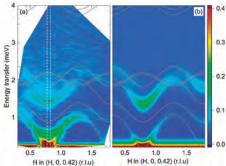


Figure 2: Results of inelastic neutron scattering: (a) measurement and (b) theoretical model.



Figure 3: In a Kitaev honeycomb magnet, a spin flip fractionalizes into three fractional quasiparticles: a Majorana fermion (red trace) and two excited gauge fluxes (blue hexagons).

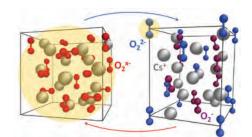


Figure 4: Charge ordering in  $Cs_4O_6$  is temperature dependent and is responsible for the change in the crystal structure and the electrical conductivity.

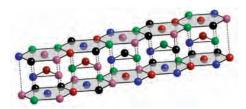


Figure 5: Schematic presentation of the crystal structure of a hexagonal high-entropy alloy, composed of five chemical elements that mix randomly on the lattice.

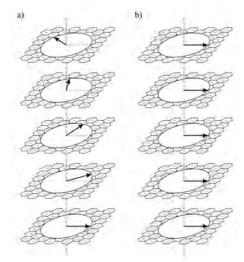


Figure 6: Schematic presentation of (a) helical antiferromagnetic structure and (b) ferromagnetic structure.

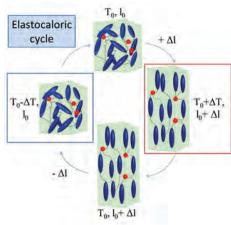


Figure 7: Elastocaloric cooling cycle.

atomic pair at this distance. Hence, we obtained direct information about the specific atomic off centring corresponding to polar vectors in real space, which was correlated with the dielectric, polarization and electrocaloric response of the lead-free relaxor system Ba(Ti,Zr)O<sub>3</sub>. The study was published in Pramanick, A., Dmowski, W., Egami, T.I, Setiadi Budisuharto, A., Weyland, F., Novak, N., Christianson, A., Borreguero, J. M., Abernathy, D., J rgensen, M. R. V. Stabilization of Polar Nanoregions in Pb-free Ferroelectrics. *Physical Review Letters* **120** (2018), 207603.

We showed by direct measurements the existence of the large electrocaloric effect in novel bulk lead-free materials. In addition, we demonstrated that these materials can replace materials based on lead due to their large electrocaloric responsivity and large breakdown electric field. A patent application, which was bought by the company Gorenje d.d. in 2016, has been awarded a USA patent in 2018: patent Malič, B., Uršič, H., Kosec, M., Drnovšek, S., Cilenšek, J., Kutnjak, Z., Rožič, B., Flisar, U., Kitanovski, A., Ožbolt, M., Plaznik, U., Poredoš, A., Tomc, U., Tušek, J.. *Method for electrocaloric energy conversion: United States Patent US9915446 (B2), 2018-03-13.* 

# 4. Enhanced electrical response in ferroelectric thin-film capacitors with inkjet-printed $LaNiO_3$ electrodes

We have developed an inkjet-printing process for lanthanum nickelate ( $LaNiO_3$ , LNO) top electrodes onto ferroelectric Pb(Zr,Ti)O<sub>3</sub> (PZT) thin films on platinized silicon substrates. The evolved ink formulation enabled the deposition of well-defined, smooth, and flat layers with minimal inter-diffusion at the LNO-PZT interface. The capacitors exhibit better polarization-switching characteristics, improved fatigue properties, and an about 40 % larger dielectric constant than those with sputtered gold top electrodes. The Rayleigh analysis of the dielectric response revealed the strongly enhanced mobility of the ferroelectric domain walls as the main contribution to improved characteristics of the LNO-PZT capacitors. Published in: A. Matavž, J. Kovač, M. Čekada, B. Malič, V. Bobnar, Applied Physics Letters 122, 214102 (2018).

# 5. Cellulose nanofibrils-reduced graphene oxide xerogels and cryogels for dielectric and electrochemical storage applications

Composites with reduced graphene oxide incorporated into the cellulose nanofibrils matrixes were fabricated as a dense film-like xerogel and well-aligned micro-to-nano porous cryogels and evaluated related to their dielectric properties and electrochemical storage capacity. An outstanding dielectric performance and high flexibility of the xerogel sample makes it a promising candidate as a highly-performing dielectric material for energy-storage applications in engineering and electronic fields. On the other hand, the high specific capacitance and electrochemical resistance indicate the suitability of porous cryogel as an electrode material in electrochemical storage devices. Published in: Y. Beeran, V. Bobnar, M. Finšgar, Y. Grohens, S. Thomas, V. Kokol, Polymer 147, 260 (2018).

# 6. Direct patterning of piezoelectric thin films by inkjet printing

We have developed a novel process for the patterning of lead zirconate titanate (PZT) films on pristine platinized silicon through the use of inkjet-printed alkanethiolate-based templates. The technique requires neither lithography nor etching, respectively, before and after PZT printing. The described process allows for feature sizes in the sub-100-µm range with control over the thickness of the final film. Inkjet-printed PZT displays the typical ferroelectric and piezoelectric properties of solution-derived thin films. Since substrate templating and functional material deposition are performed via additive manufacturing and using the same technology, we argue that our process could be an economically viable alternative to conventional deposition processes of patterned metal oxide films on high-surface-energy metal substrates. Published in: N. Godard, S. Glinšek, A. Matavž, V. Bobnar, E. Defay, Advanced Materials Technologies (2018), doi: 10.1002/admt.201800168.

## 7. Parameter optimizations for the synthesis of Al-doped ZnO nanodiscs by laser ablation in water

Al-doped ZnO crystalline colloidal nanodiscs were synthesized by the laser ablation of ZnO:Al $_2O_3$  in MilliQ water. Experiments were performed systematically by changing the number of applied laser pulses and laser output energy with the aim to affect the nanoparticle size, composition (Al/Zn ratio) and characteristics (band-gap, crystallinity). Distinctly, a set of nanoparticle syntheses was performed in deionized water for comparison. An SEM investigation of colloidal nanoparticles revealed that the formed nanoparticles are 30-nm-thick nanodiscs with average diameters ranging from 450 to 510 nm. It was found that craters in the target formed during the laser ablation influence the size of the synthesized colloidal nanoparticles. This is explained by the efficient nanoparticle growth through a

diffusion process, which takes place in the spatially restricted volume of the target crater. When laser ablation takes place in deionized water, the synthesized nanoparticles have a mesh-like structure with a sparse concentration of disc-like nanoparticles. The Al/Zn ratio and band-gap energy of the nanoparticles are highly influenced by the number and output energy of applied laser pulses (N. Krstulović, K. Salamon, O. Budimilja, J. Kovač, J. Dasović, P. Umek, I. Capan: *Applied Surface Science* 440 (2018) 916–925).

# 8. Re-Orientational Motions and Ionic Conductivity in $(NH_4)_2B_{10}H_{10}$ and $(NH_4)_2B_{12}H_{12}$

Closo-boranes are promising materials for use in solid-electrolyte fuel cells due to their high ionic conductivity. We investigated two ammonium borane systems, containing 10 or 12 boron atoms in a boron cage (Figure 9). Molecular motions were studied by means of 'H and 'B NMR spectra and spin-lattice relaxation. We identified activation energies for rotations of the boron cages around different axes. These rotations assist the long-range diffusion of  $NH_4$  units. Independent ionic conductivity measurements uncovered that these two systems are bad conductors and that the conductivity cannot be explained solely by the rotations of boron cages. Published in: Anton Gradišek, Mitja Krnel, Mark Paskevicius, Bjarne R. S. Hansen, Torben R. Jensen, Janez Dolinšek, *J. Phys. Chem. C*, 2018, 122, 17073-17079.

## 9. NMR investigations of liquid-crystalline elastomers

We investigated the orientational ordering of molecular building blocks in liquid single-crystal elastomers, using deuteron quadrupole perturbed nuclear magnetic resonance. By analysing the temperature dependencies of spin-spin and spin-lattice magnetization relaxation rates, we have resolved differences in the re-orientational dynamics of network-bound and free mesogen molecules, as well as of crosslinker molecules in selectively deuterated networks. We have found the dynamics of crosslinker to be substantially slower than the dynamics of mesogen, leading in the first case to strong homogeneous broadening of the resonance lines. This supports the scenario of substantial local disorder in the nematic director for real liquid single-crystal elastomer networks.

Research activities in the field of the physics of liquid crystal elastomers have been extended to binary systems, consisting of two mesogen species, typically of a nematogen and of a smectogen, with controlled composition. In such systems, the temperature profiles of elastic and thermomechanical response can be altered by changing the composition. We have shown that a relatively low external mechanical stress induces a transition from the smectic to the nematic state in the networks of composition close to 1:1, as observed through a decrease in the elastic constant by at least one order of magnitude (Figure 10).

Published in: Dynamic investigation of liquid crystalline elastomers and their constituentas by <sup>2</sup>H NMR spectroscopy, J. Milavec, A. Rešetič, A. Bubnov, B. Zalar, and V. Domenici, Liquid Crystals 45, 2158-2173 (2018); Stress-strain and thermomechanical characterization of nematic to smectic A transition in a strongly-crosslinked bimesogenic liquid crystal elastomer, A. Rešetič, J. Milavec, V. Domenici, B. Zupančič, A. Bubnov, and B. Zalar, Polymer 158, 96-102 (2018).

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

The investigations of the research program "*Physics of Soft Matter, Surfaces, and Nanostructures*" focus on novel complex soft-matter systems and surfaces with specific functional properties. The aim of the program is to understand the structural and dynamical properties of these systems, their interactions, their function at the molecular level, and self-assembly mechanisms in soft matter. The underlying idea is that it is possible to understand complex mechanisms, such as self-assembly, on a macroscopic level, using a simplified physical picture and

models. In order to provide a comprehensive approach to the problem, the program combines both experimental and theoretical investigations, supported by modelling and simulations. Special emphasis is given to the possible electro-optic and medical applications.

## Topological defects stabilized by fibres in a nematic liquid crystal

We demonstrate the stabilization of a large number of oppositely charged topological defects around helical colloids or grooved rods (*Soft Matter*, 14, (2018), 9819). In the case of straight fibres such defects are annihilated, but in this case the curved shape of the helical colloids or the grooved surface of a straight rod create energy barriers between neighbouring defects and prevent their annihilation. We also demonstrate a new type of topological loops

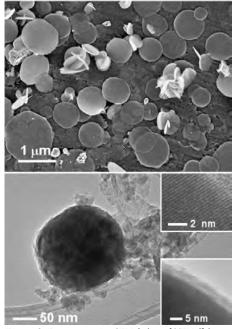


Figure 8: Representative SEM (a) and TEM (b) images of Al-doped ZnO nanodiscs. The particles were formed by irradiation of the ZnO:Al<sub>2</sub>O<sub>3</sub> target with 10,000 laser pulses and 300 mJ of laser output energy ( $\lambda_{\text{laser}}$ =1064 nm).

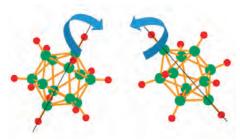


Figure 9: Structural details of  $(NH_4)_2B_{10}H_{10}$  in  $(NH_4)_2B_{12}H_{12}$  containing 10 or 12 boron atoms in a boron cage.

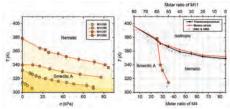


Figure 10: Temperature-composition-stress phase diagram of a binary smectic-nematic liquidcrystal elastomer.

Using numerical modelling we have identified a novel coupling mechanism that is responsible for driven passive defects in active nematic. We succeeded in generating a large number of topological defects on spiral and ribbed colloids in the nematic liquid crystal and explain the mechanism of their stabilisation. We observed strong resonances in the photo-luminiscent spectra emitted by MoS<sub>2</sub> microtubes.

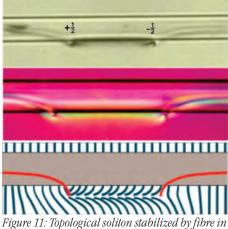


Figure 11: Topological soliton stabilized by fibre in a nematic liquid crystal.

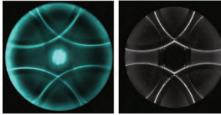


Figure 12: Experimental and numerically calculated Kosselov diagram of light reflected from a thin layer of a chiral liquid crystal forming a Skyrmion lattice.

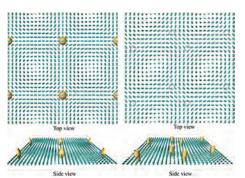


Figure 13: Periodically patterned molecular anchoring on confining surfaces stabilizes square lattices of half-Skyrmions and disclinations with winding number -1.

on a homeotropic fibre aligned perpendicular to the nematic director in a planar nematic cell. These stable loops can carry either positive or negative charge, or can be charge neutral and are always accompanied by two topological solitons, which emanate from the loop and propagate to the left- and right-hand sides of the fibre (*Liquid Crystals*, **45**, (2018) 2294).

## Observation of a Skyrmions lattice in an ultra-thin liquid-crystal layer

We identified the hexagonal lattice of half-Skyrmions in a thin film of a chiral liquid crystal by optical observation using the Kossel technique (*Scientific Reports*, 8, (2018) 17234). In the presented case Kossel lines appear as hexagonally arranged circular arcs and can be regarded as the manifestation of the dispersion eigenmodes of the medium. Our study

demonstrates that the Kossel technique could be used to investigate the dispersion properties of thin systems that exhibit non-trivial band structures such as topologically protected exotic surface states in the optical regime.

# Modelling thin layers of blue phases: stabilization of Skyrmion lattices and near-field optical microscopy

Solving Maxwell equations, we modelled optical images of Skyrmion lattices in thin layers of cholesteric blue phases that can be obtained by near-field optical microscopy. (Optics Express 26, (2018)1174). With Q-tensor-based phenomenological modelling we demonstrated how in thin layers of cholesteric blue phases of the second kind we can, with periodically patterned molecular anchoring on confining surfaces, stabilize square and trigonal lattices of half-Skyrmions (*Liquid Crystals*, 45, (2018) 2329–2340).

# Topology of chiral nematic liquid crystals

Springer published the doctorate of Gregor Posnjak as a book in the Springer Theses series (Topological formations in chiral nematic droplets) in which they publish exceptional doctoral theses. The book presents a newly developed fluorescent confocal polarized microscopy method that enables an experimental determination of the director structures in liquid crystals. This method is used to study the complex structures of chiral nematic liquid crystals in droplets in detail. These structures range from highly symmetric layered structures and structures with line defects to newly observed point defects with topological charges -2 and -3, which enable the formation of complex topological molecules.

## Localised opto-thermal response of nematic liquid crystal to laser light

We studied the non-equilibrium dynamics of the isotropic-to-nematic phase transition by observing the thermal response of a thin nematic liquid-crystal layer to a strong laser pulse, which is partially absorbed by the Indium Tin Oxide electrodes of the measuring LC cell. During the ultra-fast cooling the temperature profile of the heated region and the time response of the nematic layer birefringence were measured. (*Liquid Crystals, DOI: 10.1080/02678292.2018.1557270*).

## Active nematic emulsions

Active nematic emulsions were demonstrated based on the encapsulation of an active liquid crystal, based on microtubules and kinesin molecular motors, into a thermotropic liquid crystal. These active nematic emulsions exhibit a variety of dynamic behaviours that arise from the cross-talk between the topological defects, separately residing in the active and passive components. Using numerical simulations, we show a feedback mechanism by which active flows continuously drive the passive defects. Such a hybrid active-passive system provides new perspectives for the dynamic self-assembly driven by an active material but regulated by the equilibrium properties of the passive component. The research was a combination of numerical modelling, performed at the Faculty of Mathematics and Physics at the University of Ljubljana and the Department of Condensed Matter Physics at the Jožef Stefan Institute, and experiments, which were performed at University of Barcelona. (Science Advances 4, (2018) eaao1470).

### Read-on-demand microstructures in nematic cells

The generation of read-on-demand images and identification codes in a liquid-crystal (LC) device was demonstrated. Experimentally, these micrometre-sized polymer features are encoded directly into LC devices using direct laser writing, which locks in the local molecular orientation at the moment of fabrication. By reading the devices with the same voltage amplitude that is used to write the polymer structures, features can be made to disappear as the director profile becomes homogeneous with the surrounding regions, effectively cloaking the structure for both polarized and unpolarized light The potential use of this work is in authenticity and identification applications. Experiments were performed at the University of Oxford, whereas theory and numerical modelling were conducted at the Faculty of Mathematics and Physics at the University of Ljubljana and the Department of Condensed Matter Physics at the Jožef Stefan Institute (Advanced Optical Mater 6 (2018) 18005159). The work was also presented by the editors of Nature Photonics (Nat. Photon. **12**, (2018) 504).

## Electro-caloric effect in nematics and its applications

Using Landau-type mesoscopic modelling, we demonstrated that the materials exhibiting continuous symmetry-breaking phase transitions could be efficiently exploited for thermal stabilisation and thermal transport. In particular, we developed a pioneering model describing the electrocaloric (EC) response in nematic liquid crystals. Using it we determined the conditions enabling anomalously strong EC responses (Energy 162, (2018) 554-563).

## Nematic droplets in water solutions of different electrolytes

We demonstrated experimentally and theoretically the strong impact of the electrostatic properties on structural transitions in nematic liquid-crystal (NLC) droplets dispersed in different aqueous environments. Among others we developed a phenomenological model of an electric double layer in the presence of different ionic impurities. The results reveal that one could sensitively control the NLC structural transitions by tuning the electrostatic properties (Soft Matter 14, (2018) 9619-9630).

## Nanosafety

We measured the release of nanoparticles during the burning of incenses, which are still in use as air fresheners, for insect repelling or for meditative purposes, although it is known that they significantly deteriorate the quality of indoor air (Air Quality, Atmosphere & Health **11**, (2018) 649-663). In the case of two types of incense, we found that the burning of a single incense causes a 30-fold increase in the number of nanoparticles in a room of 30 m<sup>3</sup> volume. The chemical analysis of the released nanoparticles showed the presence of  $CaCo_3$ ,  $SiO_2$ , and traces of Mg, K, Al, Fe and Cl. At the end of the burning period, the nanoparticles are 60 to 100 nm in size, which puts them in a size group with a high health risk. The concentration exceeds 200,000 nanoparticles/cm<sup>3</sup>. Their concentration only slowly decreases with time on account of the agglomeration into larger particles. In order to reduce the exposure to nanoparticles, we recommended shortening the burning time and ventilation of the room.

## MoS2 micro- and nanotubes

In collaboration with coworkers from Russia, USA and France, we studied the optical properties of  $MOS_2$  micro- and nanotubes prepared by chemical transport reaction, which enables the growth of nanotubes with a very small concentration of structural defects. Strong peaks in the micro-photoluminescence ( $\mu$ -PL) spectra were revealed, when detecting the light polarized along the nanotube axis. (*Appl. Phys. Lett.* **113**, (2018) 101106). A model describing the optical proper-

ties of the nanotubes acting as optical resonators was developed, which supports the quantization of whispering gallery modes inside the nanotube wall. Our findings open a way to use such nanotubes as the polarization-sensitive components of nanophotonic devices.

### Self-assembly of organic corrosion inhibitors on metal surfaces

We studied (sub-)monolayers of the organic corrosion inhibitor 2-mercaptobenzimidazol on copper surfaces using scanning tunnelling microscopy and spectroscopy. By varying the substrate temperature during the deposition and using different heat treatments afterwards, we were able to study molecule-molecule and molecule-substrate interactions. The studied structures were compared and solved with the help of extensive DFT calculations. The results will help us to understand the reasons for the high effectiveness of these molecules as corrosion inhibitors.



Figure 14: A layered structure in a chiral nematic droplet with cylindrical symmetry and a single point defect.

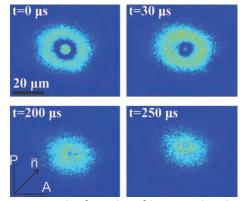


Figure 15: Ultra-fast cooling of the nematic liquid crystal.

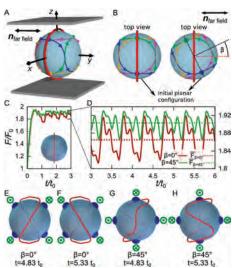


Figure 16: Coupling of the active defects to the passive nematic liquid crystal.

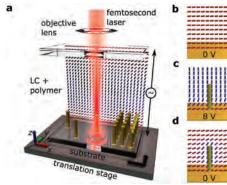


Figure 17: Direct laser writing of birefringent polymer objects that can be cloaked with birefringence.

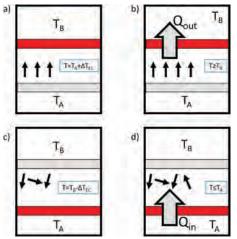


Figure 18: Key stages of the EC-based cooling cycle.

#### Structure of quasi one-dimensional charge density wave material

The basic and the charge density wave (CDW) structures of the monoclinic NbS<sub>3</sub>-II polymorph were studied by synchrotron X-ray diffraction, ab-initio calculations, simulation of the electron diffraction patterns, and by atomic-resolution transmission electron and low-temperature scanning tunnelling microscopies. By solving the structure we were able to propose a mechanism for CDW sliding that is observed in this and some related materials (Physical Review B 98, (2018) 174113).

## Atom laser and Bose fireworks

Two interesting phenomena in Bose-Einstein condensates have been observed. Firstly, if the dipole trap potential is slowly opened on the bottom, a coherent downwards flow of atoms appears – a continuous atom laser. Secondly, by periodically modulating the interatomic interaction the condensate inside a quasi-one-dimensional confinement emits jets of atoms. The simple one-dimensional geometry offers a new, simpler environment to study these so-called Bose fireworks that have previously only been observed in a two-dimensional geometry.

## Smeared d-wave anisotropy in a monolayer organic superconductor

The smeared anisotropy of low-lying quasiparticles in a single-layer d-wave organic superconductor is observed when the anti-nodal states are inextricably mixed. The weak momentum dependence is only manifested for low-lying states, while higher-energy states preserve their momentum anisotropy (Advanced Electronic Materials, DOI: 10.1002/aelm.201800247)

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

The programme group "Experimental biophysics of complex systems and imaging in biomedicine" combines research of the processes and structures of biological systems by developing new, advanced experimental techniques of super-resolution microscopies, micro-spectroscopies and nano-scopies as well as new imaging techniques. Our research is mainly focused on the response of molecular and supramolecular structures to interactions between materials and living cells as well as between light and living cells. We are interested in molecular events and the physical mechanisms with which these events are causally connected, time scales, conditions and the applied value of the investigated mechanisms, especially for use in medicine and in the field of health care in general. With the development of new, coupled super-resolution and spectroscopic techniques we want to open up new possibilities to investigate biological systems

A new molecular event has been described in our article in Nano letters, which is triggered by lipid wrapping that can drive the relocation of membranes and membrane proteins across the living pulmonary epithelium.

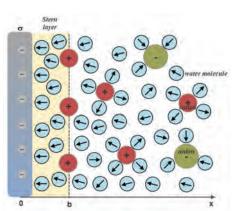


Figure 19: Schematic figure on an electric double layer near a negatively charged surface.

**described in triggered by elocation of s across the epithelium.** materials and devices, for diagnostics, therapy and tissue regeneration, representing key challenges due to the aging population. The investment into the new super-resolution STED system opened a variety of fluorescence microscopy approaches: STED microscopy and two-photon (2PE) microscopy, multichannel spectrally resolved fluorescence lifetime imaging (spFLIM), fluorescence micro-spectroscopy (FMS). These, coupled with optical tweezers, can be used to examine interactions between materials, nanomaterials and cell

and from there onwards to open up new possibilities for designing medical

lines and the phenomena involved such as lipid wrapping, membrane disintegration, and cellular membrane translocation, bypassing conventional signalling pathways. We also introduced a method that enables the monitoring of the electric field in tumours in the treatment of cancer with electroporation, and further developed a method of multiparametric magnetic resonance imaging for the characterization of food and medicines and various industrial processes. Highresolution magnetic resonance imaging can monitor the effectiveness of surface treatments, the formation and dissolution of gels as well as measure diffusion in confined geometries with the use of modulated gradients.

Because of the introduction of nonlinear super-resolution live microscopy in 2017 to monitor the changes in supramolecular structures in living systems and deep involvement in the H2020 SmartNanoTox project, in 2018 the team of the Laboratory of Biophysics successfully published its first high-impact paper after many years. In this publication (Nano Lett., 2018, 18 (8), pp 5294–5305) we directly observed the molecular event of lipid wrapping in the lung epithelium by STED microscopy, which we could previously observe only indirectly, using many other methods. This observation has triggered many other studies, including proteomics analysis, which has been done within the SmartNanoTox consortia, in particular with David Gomez's group at UCD (Dublin, Ireland) and which indicated many possible interferences between various proteins, their relocation and the known signalling cascades. The paper published in Nano letters has discussed one of those interferences, the one that potentially leads to coagulation. However, the proteomics results led us to lysosome disruption, mitochondrial network changes, and cytoskeleton degradation as well, which have been studied by live STED microscopy in 2018. Several interesting phenomena have been observed, driven by the physical affinity between the surface of the nanomaterials and the supramolecular structures, such as fibrous structures of actin and tubulin and membranes of mitochondria, endosomes and lysosomes. The team members have a focus on the dynamics, the driving forces and correlation by the known processes such as endocytosis, linear transportation within the cell and uptake into lysosomes, where the cell would try to degrade the nanoparticles, of course unsuccessfully. As a result of such physical interactions, new structures have been observed, making the complex of remnants of cell organelles and nanomaterial. More evidences are collected to prove that these structures are growing within the cells, before the cells go into the apoptotic phase.

To understand the first contact between nanomaterials and the lung's epithelial surface, the Laboratory of Biophysics team has started the development of a living copy of a lung together with a system that mimics the breathing, including the nanomaterial exposure. Here, the problem addressed in our laboratory is the rupture of the surfactant layers that separate the air in the lung and the epithelial cell layer. The nebulization of nanomaterials has been implemented on a special incubator that allows monitoring of the cell layer by STED super-resolved microscopy live during exposure. Since nanomaterial exists as individual particles as well as various aggregates, high dynamic range vertical-section microscopy has to be applied free of PSF contamination. For that purpose, the other modality of new equipment two-photon STED microscopy has been applied (at the time of purchase this was the only commercial machine of its kind in the world) and allow us to see "nano rain" in the vertical cross-section. To colocalize with surfactant proteins SP-B and SP-C the team contacted the group of Jesus Perez Gil from Univ. Madrid (Spain), which will provide us with specific labelling of the aforementioned proteins.

To track the nanoparticles in a living organism, the NPs must have a fluorescence signal. In the past year the Laboratory of Biophysics team has designed and optimized a NP labelling protocol that is suitable for metal oxides, in general, exemplified on TiO, NPs. This protocol contains an important step, for which the basic knowhow has been transferred into our laboratory from the group of Christian Eggeling from the University of Oxford (UK). This step relies on Fluorescence Correlation Spectroscopy (FCS), which can be performed also on our STED microscope. FCS is used to validate the labelling efficiency and the desorption of the probe after labelling. In addition to the labelling protocol, our team has discovered that (at least some of) the TiO<sub>2</sub> nanostructures can be imaged without labelling by gated microscopy. The trick originates in the fact that some of the TiO<sub>2</sub> structures weakly fluoresce. Usually, this fluorescence is so fast that normal detectors do not acquire enough light. In our case, the APD detectors are fast enough, providing an opportunity to catch those photons and distinguish them from other fluorescence such as autofluorescence or the one from specific labelling. This result has been recognized by the European Commission and the SmartNanoTox project officer at the SmartNanoTox midterm evaluation in September 2018 as one of the most important results in nanotoxicology-related EU projects, since it allows the tracking of TiO, nanomaterials in vitro, in vivo and ex vivo without labelling.

For efficient labelling we have designed, synthesized and tested a series of new STEDable fluorophores where we specifically aim at molecules that rearrange slowly from plasma to internal cell membranes. Two candidates have been selected for further improvements based on the stability/possible resolution and slow rate of relocation in the lipid phase. In addition, we designed new par-fluorophores for nano-temperature mapping, which aim at detecting the temperature profiles within cells, in particular within mitochondria, where higher temperatures are expected based on the evolution adaptation of mitochondria-located enzymes.

In collaboration with the Biological Physics Group at Carnegie Mellon University, Pennsylvania, USA, we have studied the phase behaviour and structure of lipid sphingomyelin (SM) model membranes using X-ray diffraction. Despite the biological significance of SMs, there is far less structural information available for SMs compared to glycerophospholipids. We have observed clear evidence of a ripple phase for egg SM as well as palmitoyl SM for a relatively

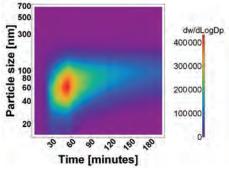


Figure 20: Number concentration of nanoparticles that are released during the burning of a single incense.

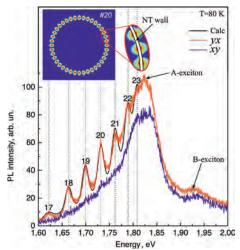


Figure 21: Micro-photoluminescence spectra ( $\mu$ PL) taken at 80 K with detecting laser light polarized along (red line) and perpendicular (blue line) to the MoS<sub>2</sub> nanotube axis. The calculated spectrum for PL is shown by the black line.

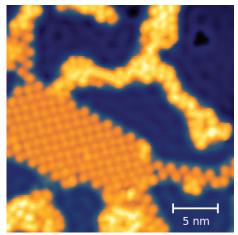


Figure 22: Ordered structures of 2-mercaptobenzimidazol molecules on a copper surface.



*Figure 23: Charge density wave and atomic structure of NbS*<sub>3</sub>-II polymorph.

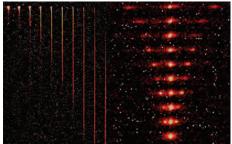


Figure 24: (Left) Atom laser from Bose-Einstein condensate of caesium atoms. (Right) Bose fireworks in a quasi-one-dimensional geometry.

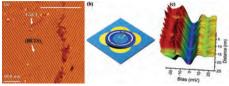


Figure 25: (a) Topographic STM image of mixed molecular orientation in a monolayer island of (BETS)<sub>2</sub>GaCl<sub>4</sub> on a Ag(111) surface. (b) Schematic representation of convoluted symmetry of superconducting gap. (c) Tunnelling spectroscopy across the line in (a) showing flat low-lying quasi particles.

broad temperature range below the main phase transition temperature. This contradicts the usual assumption that SM membranes are in the gel phase below the main phase transition. Therefore, these findings suggest the necessity to re-evaluate the interpretations of structural results obtained on physiologically relevant model lipid rafts, which contain SM as one of the lipid components. In addition, the obtained electron density profiles in the fluid phase will allow the development of improved force fields for molecular dynamics simulations.

In collaboration with the University of Oxford (UK) we showed that the activation of T cells during microscopy can only be prevented by suspending them in a hydrogel. The findings of the study involving super-resolution STED microscopy were published in Nature Immunology. Using super-resolution fluorescence correlation spectroscopy (STED-FCS) we showed that the slow diffusion of proteins in the lipid envelopes of proteins is mainly due to their composition, and not their curvature.

## Use of magnetic resonance in wood science

Magnetic resonance imaging is a very efficient method for water detection in biological systems, including wood. Water has a major influence on wood properties, especially dynamics moisture cycles, which affect wood in outdoor applications. It is therefore important to understand the penetration and distribution of water in the wood. In collaboration with colleagues from the Department of Biotechnical Faculty, University of Ljubljana, we conducted a study in which rainfall events were simulated to correspond to water-immersion periods of one hour. For the study the most important wood species in Central Europe with different water-repellent properties were used. After the immersion, the samples were imaged by MRI. Measurements were used to determine the water distribution in the wood and to elucidate the changes during the drying of the specimens. From these measurements a scientific article was published: Mojca Žlahtič Zupanc, Urša Mikac, Igor Serša, Maks Merela, Miha Humar. Water distribution in wood after short term wetting. Cellulose, ISSN 0969-0239, First Online 09 November 2018, https://doi.org/10.1007/s10570-018-2102-y.

## Use of magnetic resonance in battery research

Due to the increasing number of mobile devices, the development of more powerful batteries is necessary. Magnetic resonance imaging (MRI) can be used to monitor the growth of dendrites in batteries, and by using a special MRI technique, CD-MRI, also to monitor the electric current during battery operation. However, batteries contain metal parts (electrodes) that cause distortion of the MR image. Therefore, the influence of metal electrodes on the MRI signal in different orientations with respect to static and radio-frequency magnetic fields was tested on a

model battery, and the optimal orientation of the electrodes in which the distortions are practically negligible was determined. The results were published in the article: Igor Igor, Mikac Urka. A study of MR signal reception from a model for a battery cell. Journal of magnetic resonance, ISSN 1090-7807, 2018, 294, p. 7-15.

## Deformation tensor imaging by magnetic resonance

Magnetic resonance imaging enables the precise detection of phase changes. This, among other effects, also enables the measurement of very small displacements in the direction of the applied magnetic field gradient. In the magnetic resonance imaging laboratory we have shown that by the use of the spin-echo imaging method with a superimposed bipolar gradient pair (the PGSE method) displacements can be measured with accuracy of up to

 $0.7 \mu m$ . With experiments of the test sample, we showed that this method also enables imaging of the deformation tensor. These results were published in the article Serša Igor. Magnetic resonance imaging of strain in elastic gels. Journal of Applied Physics, ISSN 0021-8979, 2019, 125(8), p. 0825211–082521-9.

## Simulations of translational dynamics of chain-like particles through mucosal scaffolds

Mucus scaffolds represent one of the most common barriers in targeted drug delivery and can remarkably reduce the outcome of pharmacological therapies. Understanding the transport mechanism is particularly important for the treatment of disorders such as cystic fibrosis. In the study, we employed the bond fluctuation model (BFM) to analyse the effect of steric interactions on slowing the translational dynamics of compound chain-like particles, traversing through scaffolds of different configurations. The developed mathematical model accounted for the geometry-imposed steric interactions as well as for the intra-chain steric interactions between

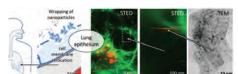


Figure 26: Causal connection has been identified between the inhalation of nanoparticles (red), lipid (green) wrapping and triggering of the coagulation signal cascade in lung epithelium, where the key experiments have been done using a super-resolution STED microscope and with TEM microscopy (IJS, Ljubljana, Slovenia) and new proteomics techniques at UCD (Dublin, Ireland). The work was published in Nano Letters.

the chain subunits. The presented model is generic and could also be applied for studying the translational dynamics of other particles with more complex architecture, such as dendrites or chain-decorated nanoparticles. The results of the study were published in Bajd Franci, Serša Igor. A bond-fluctuation model of translational dynamics of chain-like particles through mucosal scaffolds. *Biophysical journal*, ISSN 0006-3495, 2018, 114(11), p. 2732-2742.

The research at our department 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 2018, the department had cooperations with 108 partners from Slovenia and abroad. Among them:

- The high magnetic field centres in Grenoble, France, and Nijmegen, The Netherlands
- The high magnetic field centre at the University Florida, Tallahassee, Florida, USA
- The ETH, Zürich, Switzerland
- The Ioffe Institute in St. Petersburg, Russia
- The University of Duisburg, the University of Mainz and the University of Saarbrucken in Germany
- The University of California, the University of Utah and the Liquid Crystal Institute, Kent, Ohio, USA
- National Institute for Research in Inorganic Materials, Tsukuba, Japan
- NCSR Demokritos, Greece
- Institut für Biophysik und Nanosystemforschung OAW, Graz, Austria
- Bioénergétique et Ingénierie des Protéines, CNRS Marseille, France
- Architecture et Fonction des Macromolécules Biologiques, CNRS Marseille, France
- The Max Delbruck Center for Molecular Medicine in Berlin
- The Dartmouth Medical School, Hanover, NH, USA
- The Mayo Clinic, Rochester, USA
- 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 2018

- N. Janša, A. Zorko, M. Gomilšek, M. Pregelj, K.W. Krämer, D. Biner, A. Biffin, C. Rüegg, M. Klanjšek. Observation of two types of fractional excitation in the Kitaev honeycomb magnet. *Nature Physics* 14, (2018), 786-790.
- 2. P. Adler, P. Jeglič, T. Knaflič, M. Komelj, D. Arčon, et al. Verwey-type charge ordering transition in an open-shell p-electron compound. *Science Advances* 4, (2018), eaap7581.
- 3. S. Gao, S. Vrtnik, J. Luzar, et al. Dipolar spin ice states with a fast monopole hopping rate in CdEr<sub>x</sub>X<sub>4</sub> (X=Se, S). *Physical Review Letters* **120** (2018), 137201.
- Yu.O. Zagorodniy, B. Zalar et al. Chemical disorder and <sup>207</sup>Pb hyperfine fields in the magnetoelectric multiferroic Pb(Fe<sub>1/2</sub>Sb<sub>1/2</sub>)O<sub>3</sub> and its solid solution with Pb(Fe<sub>1/2</sub>Nb<sub>1/2</sub>)O<sub>3</sub>. *Physical Review Materials* 2 (2018), 014401.
- 5. J. Dolinšek. Electronic transport properties of complex intermetallics. *Crystal growth of intermetallics*, Eds. P. Gille, Yu. Grin (Berlin: De Gruyter, 2018), 260-278.
- Pramanick, A., Dmowski, W., Egami, T.I, Setiadi Budisuharto, A., Weyland, F., Novak, N., Christianson, A., Borreguero, J. M., Abernathy, D., Jørgensen, M. R. V.. Stabilization of Polar Nanoregions in Pb-free Ferroelectrics. *Physical Review Letters* 120 (2018), 207603.
- Guillamat, Pau, Kos, Žiga, Hardoüin, Jérôme, Ignés-Mullol, Jordi, Ravnik, Miha, Sagués, Francesc. Active nematic emulsions. *Science Advances* 4 (2018), 2375-2548.
- Urbančič, Iztok, Garvas, Maja, Kokot, Boštjan, Majaron, Hana, Umek, Polona, Škarabot, Miha, Arsov, Zoran, Koklič, Tilen, Čeh, Miran, Muševič, Igor, Štrancar, Janez, et al. Nanoparticles can wrap epithelial cell membranes and relocate them across the epithelial cell laye. *Nano Letters* 18 (2018), 5294-5305.
- 9. Aničić, Nemanja, Vukomanović, Marija, Koklič, Tilen, Suvorov, Danilo. Fewer defects in the surface slows the hydrolysis rate, decreases the ROS generation potential, and improves the Non-ROS antimicrobial activity of MgO. *Small* 14 (2018), 1800205.

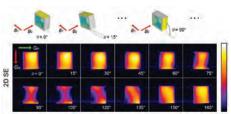


Figure 27: Effect of the model battery orientation with respect to the  $B_0$  and  $B_1$  fields on the signal suppression. As shown by the inset above the MR images, the model sample was rotated in steps on 15° around the axis parallel to the  $B_0$  field from  $\theta =$ 0° to  $\theta = 165^\circ$ . In the initial orientation ( $\theta = 0^\circ$ ) the electrodes are parallel to the  $B_1$  field so that there is no RF-induced eddy currents. As  $\theta$  is increased RF-induced eddy currents start to appear. These lead to a more extensive signal suppression that is the strongest at  $\theta = 90^\circ$  (the  $B_1$  field perpendicular to the electrodes) and diminishes again when  $\theta$ approaches 180°.

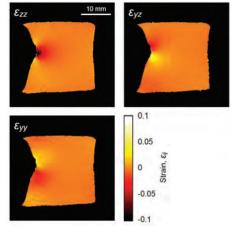


Figure 28: Maps of the three components of the strain tensor,  $\varepsilon_{yy}$ ,  $\varepsilon_{zz}$ , and  $\varepsilon_{yz}$ . The strain tensor components were calculated from maps of displacements  $u_z$  and  $u_y$ , which were obtained from images of the signal phase change induced by the sample displacements.



10. Santos, Ana Mafalda, Urbančič, Iztok, et al. Capturing resting T cells: the perils of PLL. *Nature Immunol*ogy **19** (2018), 203-205.

#### Some outstanding publications in 2017

- M. Klanjšek, A. Zorko, R. Žitko, J. Mravlje, Z. Jagličić, P.K. Biswas, P. Prelovšek, D. Mihailović, D. Arčon. A high-temperature quantum spin liquid with polaron spins. *Nature Physics* 13 (2017), 1130–1134.
- Y. Takabayashi, M. Menelaou, H. Tamura, N. Takemori, T. Koretsune, A. Štefančič, G. Klupp, A.J.C. Buurma, Y. Nomura, R. Arita, D. Arčon, M.J. Rosseinsky, K. Prassides. σ-electron S = 1/2 quantum spin-liquid state in an ionic polyaromatic hydrocarbon. *Nature Chemistry* 9 (2017), 635–643.
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- A. Zorko, M. Herak, M. Gomilšek, J. van Tol, M. Velázquez, P. Khuntia, F. Bert, P. Mendels. Symmetry reduction in the quantum Kagome antiferromagnet Herbertsmithite. *Physical Review Letter* 118 (2017), 017202.
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- S. M. Hasheimi, U. Jagodič, M. R. Mozaffari, M. R. Ejtehadi, I. Muševič, and M. Ravnik, Fractal nematic colloids. *Nature Communications* 8 (2017), 12106.
- G. Posnjak, S. Čopar and I. Muševič. Hidden topological constellations and polyvalent charges in chiral nematic droplets. *Nature Communications* 8 (2017), 14594.
- A. Nych, Jun-ichi Fukuda, U. Ognysta, S. Žumer, I. Muševič. Spontaneous formation and dynamics of half-skyrmions in a chiral liquid-crystal film. *Nature Physics* 13 (2017), 1215.
- E. Sezgin, F. Schneider, V. Zilles, I. Urbančič, E. Garcia, D. Waithe, A.S. Klymchenko, C. Eggeling. Polarity-Sensitive Probes for Superresolution Stimulated Emission Depletion Microscopy. *Biophysical Journal* 113 (2017), 1321-1330.
- M. Kranjc, S. Kranjc, F. Bajd, G. Serša, I. Serša, D. Miklavčič. Predicting irreversible electroporation-induced tissue damage by means of magnetic resonance electrical impedance tomography. *Scientific Reports* 7 (2017), 1-10.

#### Some outstanding publications in 2016

- A. Rešetič, J. Milavec, B. Zupančič, V. Domenici, B. Zalar. Polymer-dispersed liquid crystal elastomers. *Nature Communications* 7 (2016), 13140.
- M. Jeong, M. Klanjšek et al. Dichotomy between attractive and repulsive tomonaga-luttinger liquids in spin ladders. *Physical Review Letters* 117 (2016), 106402.
- 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 (2016), 10413.
- 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 (2016), 26629.
- M. Igarashi, P. Jeglič, A. Kranjc, R. Žitko, T. Nakano, Y. Nozue, D. Arčon. Metal-to-insulator crossover in alkali doped zeolite. *Scientific Reports* 6 (2016), 18682.
- G. Posnjak, S. Čopar, I. Muševič. Points, skyrmions and torons in chiral nematic droplets. *Scientific Reports* 6 (2016), 26361.
- 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. *Proceedings of the National Academy of Sciences of the United States of America* 113 (2016), 1174.
- S. Nizamoglu, M. Humar et al. Bioabsorbable polymer optical waveguides for deep-tissue photomedicine. *Nature Communications* 7 (2016), 10374.
- S. Cho, M. Humar, N. Martino, S. H. Yun. Laser Particle Stimulated Emission Microscopy. *Physical Review Letter* 117 (2016), 193902.
- 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. *Proceedings of the National Academy of Sciences of the United States of America* 113 (2016), E6582.

#### Annual Report 2018

#### Awards and appointments

1. Bizjak Jani, Gradišek Anton, Gams Matjaž: the award for the best innovation for a public research organization, Ljubljana, The 11th International Technology Transfer Conference, The ultimate European assistant for the elderly

#### Organization of conferences, congresses and meetings

- 1. The 8<sup>th</sup> Regional Biophysics Conference 2018, Zreče, 16–20 May 2018
- 2. 11th conference on fundamental physical research, Terme Dobrna, 23 November 2018
- 3. Expert meeting F-5, Orehov gaj, 10 December 2018

#### Patents granted

- 1. Andraž Rešetič, Jerneja Milavec, Blaž Zupančič, Boštjan Zalar, Polymer dispersed liquid crystal elastomers (PDLCE), US9969847 (B2), US Patent and Trademark Office, 15. 05. 2018.
- Barbara Malič, Hana Uršič, Marija Kosec, Silvo Drnovšek, Jena Cilenšek, Zdravko Kutnjak, Brigita Rožič, Uroš Flisar, Andrej Kitanovski, Marko Ožbolt, Uroš Plaznik, Alojz Poredoš, Urban Tomc, Jaka Tušek, Method for electrocaloric energy conversion, US9915446 (B2), US Patent and Trademark Office, 13. 03. 2018.

### INTERNATIONAL PROJECTS

- MERCK AFM Investigations Prof. Miha Škarabot Merck Kgaa
- 2. Kimberly-Clark Development of LCD Shutter in the Year 2018 Prof. Igor Muševič
- Kimberly-clark 3. 7FP - SIMDALEE2; Sources, Interaction with Matter Detection and Analysis of Low Energy Electrons 2
  - Prof. Maja Remškar European Commission
- 7 FP; ERA CHAIR ISO-FOOD Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability
  - Prof. Maja Remškar European Commission
- 5. COST MP1308; Towards Oxide Based Electronics (TO-BE) Aleksander Matavž
- 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
- Institut Jožef Stefan
  COST CA16109; Chemical On-Line Composition and Source Apportionment of Fine Aerosol
  - Asst. Prof. Griša Močnik
- Cost Office
- COST CA16218; Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies Dr. Abdelrahim Ibrahim Hassanien
  - Cost Office
- 10. COST CA16221; Quantum Technologies with Ultra-Cold Atoms Dr. Peter Jeglič
  - Cost Association Aisbl
- Training School on Black and Brown Carbon Organisation of the Workshop of Project COST - COLOSSAL, COST CA16109, Ljubljana, Slovenia, 15.01.-17.01.2018 Asst. Prof. Griša Močnik Cost Office
- COST CA17121; Correlated Multimodal Imaging in Life Sciences Prof. Janez Štrancar
- Cost Association Aisbl 13. COST CA17139; European Topology Interdisciplinary Action Prof. Slobodan Žumer
- Cost Association Aisbl
- COST CA16202; International Network to Encourage the Use of Monitoring and Forecasting Dust Products Asst. Prof. Griša Močnik Cost Association Aisbl
- H2020 SmartNanoTox; Smart Tools for Gauging Nano Hazards Prof. Janez Štrancar European Commission

- 16. H2020 ENGIMA; Engineering of Nanostructures with Giant Magneto-Piezoelectric and Multicaloric Functionalities
- Prof. Zdravko Kutnjak European Commission
- 17. Crystal and Electronic Structure of NbS3 Phases Dr. Erik Zupanič
- Slovenian Research Agency
- Lead-Free (Ba0.8Ca0.2)1-xLa2x/3TiO3 Based Electrocaloric Materials for New Dielectric Cooling Technologies Prof. Zdravko Kutnjak
  - Slovenian Research Agency
- 9. Stabilisation of Networks of Topological Defects
- Prof. Samo Kralj Slovenian Research Agency
- Superconductivity and Magnetism: Two Faces of Electron Correlations in Carbon- and Fe-Based Superconductors Prof. Denis Arčon
  - Slovenian Research Agency
- Transport and Field Emission Properties of Low-Dimensional Molybdenum and Tungsten Based Nanomaterials Prof. Maja Remškar
  - Slovenian Research Agency
- Testing Biocompatibility of Molybdenum and Tungsten based Nanoparticles: Measuring Cytotoxicity and Inflammatory Response in Human Cell Lines Prof. Maja Remškar
  - Slovenian Research Agency
- 23. The Lipid-Peroxidation Inhibition Governed by Interactions between Nanocarried Flavonoids and Model Lipid Membranes Prof. Janez Štrancar
  - Slovenian Research Agency
- 24. Dynamic Hysteresis in the Study of Magnetic Nanoparticle Efficacy for Hyperthermia Therapy
  - Prof. Janez Dolinšek Slovenian Research Agency
- Conservation of Cultural Heritage Indoors The Case of Leonardo da Vinci's "Last Supper"
  - Asst. Prof. Griša Močnik
- Slovenian Research Agency 26. Lipid Wrapped Nanoparticles and Activity of Factor Xa
- Dr. Tilen Koklič
- Slovenian Research Agency 27. Studies of Nanoporous Materials for Hydrogen Storage Prof. Janez Dolinšek
- Slovenian Research Agency
- 28. Magnetoresonance Study of Spin-Liquid Candidates Asst. Prof. Andrej Zorko
- Slovenian Research Agency
   Advanced Organic and Inorganic Thin-Film Composites with Enhanced Dielectric and Electromechanical Response
   Prof. Zdravko Kutniak
- Slovenian Research Agency

## RESEARCH PROGRAMS

- Magnetic resonance and dielectric spectroscopy of "smart" new materials 1. Prof. Janez Dolinšek
- 2. Physics of Soft Matter, Surfaces and Nanostructures Prof. Slobodan Žumer
- Experimental Biophysics of Complex Systems 3. Prof. Janez Štrancar

## R & D GRANTS AND CONTRACTS

- 1. High-Entropy Alloys
- Dr. Stanislav Vrtnik
- 2. Metamaterials from liquid crystal colloids
- Prof. Miha Ravnik
- Sensor technologies in diagnostics and monitoring of cultural heritage buildings 3. Prof. Janez Dolinšek
- 4. Electroporation-based treatments with new high-frequency electroporation pulses Prof. Igor Serša
- Multifunctional materials for actuator and cooling devices 5. Prof. Zdravko Kutnjak
- 6. Correlated electrons in cnofined molecular systems Prof. Denis Arčon
- High-resolution optical magnetometry with cold cesium atoms Dr. Peter Jeglič
- 8. Integrated multi-channel artificial nose for vapor trace detection Prof. Igor Muševič
- Photonic devices made entirely out of edible materials Asst. Prof. Matjaž Humar
- 10 Probing spin states near the surface of quantum spin materials Prof. Denis Arčon
- Advanced soft nematocaloric materials 11.
- Dr. Brigita Rožič 12
- Multicaloric cooling Prof. Zdravko Kutnjak

### VISITORS FROM ABROAD

- Dr Hashemi Masoomeh, Sharif University of Technology, Tehran, Iran, 1 November 1. 2017 to 31 January 2018, 4 February to 30 March 2018 and 1-28 April 2018
- 2. Patrycja Boguslawa Zawilska, Faculty of Biotechnology, University of Wroclaw, Wroclaw, Poland, 7–28 January 2018 and 16 April to 16 June 2018
- Prof. Katsumi Tanigaki, Materials Physics and Nano Solid-State Physics, Tohoku 3. University, Sendai, Japan, 28-30 January 2018
- Dr Nych Andriy, Institute of Physics, Kiev, Ukraine, 22 January to 2 February 2018 4
- Takuma Ogasawara, Materials Physics and Nano Solid-State Physics, Tohoku University, 5. Sendai, Japan, 28 January to 23 February 2018
- Prof. Stoeger Tobias and Dr Mendes Carola, Helmholtz Center Munich, Institute of Lung 6 Biology and Disease, Munich, Germany, 18-22 March 2018
- 7. Prof. Makan Wallin, National Institute of Occupational Health, Oslo, Norway, 18-23 March 2018
- 8 Dr Mendels Philippe, Laboratoire de Physique des Solides, Universite Paris-Sud, Orsay, France, 28-29 March 2018
- Prof. Dr Hoet Peter, KU Leuven, Department of Public Health and Primary Care, Centre 9 Environment and Health, Leuven, Belgium, 9-10 April 2018
- 10. Prof. Dr Guo Sheng, Chalmers University of Technology, Gothenburg, Sweden, 15-18 April 2018
- 11. Dr Šegota Suzana and Dr Baranović Goran, Ruđer Bošković Institute, Zagreb, Croatia, 28 May to 1 June 2018
- 12. Prof. Dr Smalyukh Ivan, University of Colorado, Boulder, Colorado, USA, 1 June 2018
- 13. Dr Kimouche Amina, School of Science, Aalto University, Helsinki, Finland, 14-21 June 2018 14. Dr Dhara Surajit, School of Physics, University of Hyderabad, Hyderabad, India, 16 June
- to 7 July 2018 15. Dr Ryzhkova V. Anna, ASML, Eindhoven, the Netherlands, 9-15 July 2018 and 21
- October to 10 November 2018 16. Prof. Dr Kotur Bogdan, Ivan Franko National University of Lviv, Lviv, Ukraine, 14-17
- July 2018
- Dr Ositi Agnese, Faculty of Chemistry, University of Latvia, Riga, Latvia, 2-7 July 2018 Dr Majhen Dragomira and Nestić Davor, Ruđer Bošković Institute, Zagreb, Croatia, 13 18. July 2018
- Dmitry Richter, Ruprecht-Karls-Universität Heidelberg, Heidelberg, Germany, 15 July-15 19. August 2018 and 8 September to 31 October 2018
- 20. Dr Asbani Bouchra, Université de Picardie Jules Verne, Laboratoire de Physique de la Matière Condensée, Amiens, France, 29 July to 7 August 2018
- Hajar Zaitouni, University Cadi Ayyad, Marrakesh, Morocco, 29 July to 4 September 2018
- 22. Dr Abdelhadi Alimousa, University Cadi Ayyad, Marrakesh, Morocco 3-18 August 2018
- 23. Prof. Mezzane Daoud, University Cadi Ayyad, Marrakesh, Morocco, 13-31 August 2018 24. Prof. Schreiner Rupert, Lawrowski Robert, Assist. Prof. Huettel Andreas and Reinhardt

- 13. Optimization of MRI techniques for assessment of thrombolytic treatment outcome Prof. Igor Serša
- 14. Performance of wood and lignocelolosic composites in outdoor applications Prof. Igor Serša
- 15. Advanced electrocaloric energij conversion Prof. Zdravko Kutnjak
- Biopharmaceuticals: sensor for aggregation of protein particles based on liquid crystals 16. Prof. Miha Ravnik
- 17. Spatial and temporal shaping of laser light for minimally invasive ophthalmic procedures
- Prof. Janez Štrancar 18. Microspectroscopy-based optimization of the effects of laser pulses on the retina Prof. Janez Štrancar
- Domain engineered ferroelectric ceramic layer elements for efficient energy harvesting 19. and energy conversion applications Prof. Zdravko Kutnjak
- Building blocks, tools and systems for the Factories of the Future GOSTOP Prof. Janez Štrancar
- Ministry of Education, Science and Sport
- 21. Irradiation and Analysis of Nano SiC Samples in the Year 2017 Prof. Vid Bobnar National Nuclear Research Center
- Inkjet Printing of PZT Test Structures and Piezoelectric Characterization of Thin Films Double-Beam Laser Interferometer Measurement Prof. Vid Bobnar Epcos Ohg

### NEW CONTRACTS

- Instrumentation for measurement of aerosol light absoption 1. Prof. Igor Muševič Ames d. o. o.
- Detecion of Non-Anthropogenic Air Pollution project (DNAAP) Asst. Prof. Griša Močnik Aerosold o o
  - Simon, Institute for Experimental and Applied Physics, Regensburg, Germany, 15-18 August 2018
- 25. Dr Wencka Magdalena, Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland, 19-31 August 2018
- 26. Dr Savić Aleksandar, Institute for Multidisciplinary Research, Beograd, Serbia, 20-31 August 2018
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- 29. Dr Kimouche Amina, Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain, 24 September to 6 October 2018
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# DEPARTMENT FOR COMPLEX MATTER

**F-7** 

The research within the Department of Complex Matter encompasses a variety of research fields, ranging from the synthesis of new materials to fundamental investigations of elementary excitations in complex systems: from nano-biosystems to exotic magnetic systems and superconductors. The experimental methods used are suitably diverse, from synthetic chemistry to femtosecond laser spectroscopy. The 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 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 the fields of quantum molecular electronics and nanoelectronics. These and other materials, such as strongly correlated systems, electronically ordered systems and superconductors were investigated using advanced femtosecond spectroscopy techniques. In a number of areas we Head: have introduced new materials, technologies and techniques.



Prof. Dragan D. Mihailović

#### Ultrafast studies of electron and lattice dynamics in complex 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 collec- European Research Council tive excitations under extreme conditions, such as those arising from strong and selective photo-stimulation. These Established by the European Commission developments are opening the way for new, non-equilibrium phenomena that can eventually be induced and manipulated by short laser pulses.

The optical control of states exhibiting macroscopic phase coherence in condensed-matter systems opens intriguing possibilities for materials and device engineering, including optically controlled qubits and photo-induced superconductivity. Metastable states, which in bulk materials are often associated with the formation of topological defects, are of more practical interest. Scaling to nanosize leads to reduced dimensionality, fundamentally changing the system's properties. In one-dimensional superconducting nanowires, vortices that are present in threedimensional systems are replaced by fluctuating topological defects of the phase. These drastically change the dynamical behaviour of the superconductor and introduce dynamical, periodic long-range ordered states when the current is driven through the wire. We report on the control and manipulation of transitions between different dynamically stable states in superconducting  $\delta_{a}$ -MoN nanowire circuits by ultrashort laser pulses. Not only can the transitions between different dynamically stable states be precisely controlled by light, but we also discovered new photoinduced hidden states that cannot be reached under near-equilibrium conditions, created while laser photoexcited quasi-particles are outside the equilibrium condition. The observed switching behaviour can be understood in terms of the dynamical stabilization of various spatiotemporal periodic trajectories of the order parameter in the superconductor nanowire, providing means for the optical control of the superconducting phase with sub-picosecond control of the timing. The results were published in Sci. Adv. 4, eaao0043 (2018).

The properties of strongly correlated materials originate from intertwined microscopic interactions that are hard to disentangle at equilibrium. Employing nonequilibrium, timeresolved photoemission spectroscopy in the two-dimensional transition-metal dichalcogenide



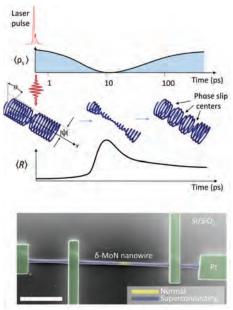


Figure 1: The appearance of superconducting phase slips of the order parameter in δ-MoN nanowires after excitation by a laser pulse.

In a combined experimental-theoretical tour-deforce described in the publication by Madan et al. (Sci. Adv. 2018), the superconducting phase slips along a  $\delta$ -MoN nanowire were controlled by short laser pulses, giving rise to quantized changes in resistance along the wire. Not only can the transitions between different dynamically stable states be precisely controlled by light, but we also discovered new photo-induced hidden states that cannot be reached under near-equilibrium conditions, created while laser photoexcited guasiparticles are outside the equilibrium condition. The observed switching behavior can be understood in terms of the dynamical stabilization of various spatiotemporal periodic trajectories of the order parameter in the superconductor nanowire, providing means for the optical control of the superconducting phase with sub-picosecond control of the timing.

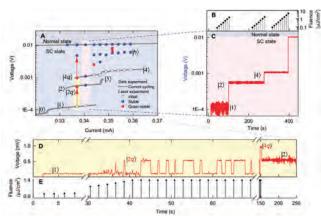


Figure 2: Optical switching to the stable and quasi-stable superconducting states in a superconducting 8-MoN nanowire.

17TaS<sub>2</sub>, we identified a signature of doubly occupied sites (doublons) that reflects fundamental Mott physics. Doublon-hole recombination is estimated to occur on timescales of electronic hopping  $\hbar/J \approx 14$  fs. Despite strong electron-phonon coupling, the dynamics can be explained by purely electronic effects captured by the single-band Hubbard model, as reported in Phys. Rev. Lett. 120, 166401 (2018).

The transition to a hidden metastable state in 17-TaS<sub>2</sub> is investigated in real time using coherent time-resolved femtosecond spectroscopy. Relying on spectral differences between the phonon modes in the equilibrium states and in the metastable state, and temperature-tuning the metastable state lifetime, we perform stroboscopic measurements of the electronic response and switching of the coherent oscillation frequency through the transition. Very fast coherent switching of the collective-mode frequency is observed (~400 fs), comparable to the electronic time scale of ~300 fs. The observations are described well by a fast electronic band-structure transformation into the metastable state, consistent with a topological transition. The results were published in **Phys. Rev. B** 97, 075304 (2018).

Femtosecond transient optical spectroscopy was also employed to study the relaxation dynamics of the equilibrium and hidden metastable charge-density-wave states in single crystals of  $17^{2}\text{TaS}_{2-x}\text{Se}_{x}$  as a function of the Se doping *x*. Similar to pristine  $17^{2}\text{TaS}_{2}$ , the transition to a hidden phase is observed at low temperature after a quench with a single 50 fs laser pulse, in the commensurate Mott phase up to x = 0.6. The photo-induced hidden-phase formation is accompanied by a notable change in the coherent phonon spectra, and particularly the collective amplitude mode. While the temperature stability of the hidden phase is only slightly dependent on the Se content, the creation-threshold fluence strongly increases with Se content from 1 to ~4 mJ/cm<sup>2</sup>, which is attributed predominantly to the change in optical absorption coefficient at the laser excitation wavelength, and not an increased barrier of the hidden state with increasing This was reported in Phy. Rev. B 98, 195121 (2018).

New emergent states of matter in quantum systems can be created under non-equilibrium conditions if – through many-body interactions – its constituents order on a timescale that is shorter than the time required for the system to reach thermal equilibrium. Conventionally non-equilibrium ordering is discussed in terms of symmetry breaking, nonthermal orderdisorder, and more recently quenched topological transitions. Here we report a fundamentally new and unusual metastable form of amorphous

correlation-localized fermionic matter, which is formed in a new type of quantum transition at low temperature either by short pulse photoexcitation or by electrical charge injection in the transition-metal dichalcogenide  $17^{-}$ TaS<sub>2</sub>. Scanning tunnelling microscopy (STM) reveals a pseudo-amorphous packing of localized electrons within the crystal lattice that is significantly denser than its hexagonally ordered, low-temperature ground state, or any other ordered states of the system. Remarkably, the arrangement is not random, but displays a hyperuniform spatial density distribution commonly encountered in classic jammed systems, showing no signs of aggregation or phase separation. Unexpectedly for a localized electron system, tunnelling spectroscopy and multi-STM-tip surface resistance measurements reveal that the overall state is gapless and conducting, which implies that localized and itinerant carriers are resonantly entangled. The amorphous localized electron subsystem can be understood theoretically to arise from strong correlations between polarons sparsely dispersed on a 2D hexagonal atomic lattice, while itinerant carriers act as a resonantly coupled reservoir distinct in momentum space. The manuscript is currently under review, and the latest preprint can be found at **arXiv:1803.00255**.

The search for a metastable state switched by ultrafast laser pulses or electrical pulses has led to several patent applications and international projects and collaborations.

#### 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-TaS<sub>2</sub> to a metastable electronic state with textured domain walls, accompanied by the conversion of polarons

#### We have discovered the possibility of hyperuniform ordering in electronic systems.

to band states, and concurrent rapid switching from an insulator to a metal. The large resistance change, high switching speed (30 ps) and ultra-low energy per bit opens the way to new concepts in non-volatile memory devices manipulating all-electronic states.

#### Quantum jamming transition to a correlated electron glass in 1T-TaS<sub>2</sub>

Different many body states can be created under non-equilibrium conditions through different ordering paths, even when their constituents are subject to the same fundamental interactions. In spite of significant recent interest, only very few truly exotic emergent states have been discovered to date, and even fewer have been satisfactorily elucidated. So the phase transition mechanisms to such emergent states are still poorly understood. Here we show that controlled optical or electromagnetic perturbations can lead to an unusual amorphous metastable state of

strongly correlated electrons in a quasi-two-dimensional dichalcogenide 1T-TaS<sub>2</sub>. Scanning tunnelling microscopy reveals a "hyper-uniform" pattern of localized charges arranged in a mosaic of differently charged tiles. Unexpectedly for localized charges, multi-tip surface nanoscale conductivity measurements and tunnelling spectroscopy show an electronically gapless conducting state that is different from conventional Coulomb glasses and many-body localized systems. Relaxation measurements show that the state is stable up to room temperature and shows no signs of either local charge order or phase separation. The mechanism for its formation is attributed to a dynamical localization of electrons through mutual interactions. Theoretical calculations confirm the correlations between localized charges to be crucial for the state's unusual stability. Preprint can be found at **arXiv: 1803.00255**.

## Mottness collapse without metallization in the domain wall of the triangular-lattice Mott insulator 1T–TaS<sub>2</sub>

1T—TaS2 is a charge-density-wave (CDW) compound with a Mottinsulating ground state. The metallic state obtained by doping, substitution, or pulsed charge injection is characterized by an emergent CDW domainwall network, while single-domain walls can be found in the pristine Mott state. Here we study whether and how the single walls become metallic. Tunnelling spectroscopy reveals the partial suppression of the Mott gap and the presence of in-gap states strongly localized at the domain-wall sites. Using the real-space dynamical mean-field-theory description of the strongly correlated quantum-paramagnet ground state, we show that the local gap suppression follows from the increased hopping along the connected zigzag chain of lattice sites forming the domain wall. Furthermore, we show that full metallization is preempted by the splitting of the quasiparticle band into bonding and antibonding subbands due to the structural dimerization of the wall, explaining the presence of the in-gap states and the low density of the states at the Fermi level. Sumbitted to **Phys. Rev. Lett.** 

#### Spectroscopic equilibrium and time-resolved studies of the electronic structure of the CDW molybdenum oxide Mo<sub>s</sub>O<sub>32</sub>

Recently, we have demonstrated the switching of a  $M_{0_{23}}^{0}$  single crystal into a new, long-lived metastable state that persists up to 350 K by a single ultrashort optical pulse. Only two compounds have been previously reported to demonstrate such long-lived metastable phases obtained by a single optical pulse: 1T-TaS<sub>2</sub> and strained manganite films and the underlying physics appears to be quite different: interplay of electron-lattice coupling with Mott gap collapse in the first case and with magnetic-lattice coupling

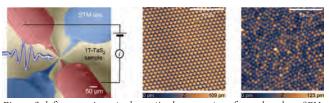


Figure 3: left – experiment schematic shown on top of pseudo-colour SEM image; center – STM image of the ground state (C) at 5K; right – STM image of the photo-induced amorphous jammed state (A) at 5K obtained with a single laser pulse of  $\sim 4mJ/cm^2$  fluence, 30 fs duration and 400 nm central wavelength.

We have observed that strong electron-electron interactions can lead to the counterintuitive behaviour of nanoscale objects like domain walls, thus paving the way to tailoring material properties in complex systems via nanomodification with the help of electrical or optical pulses.

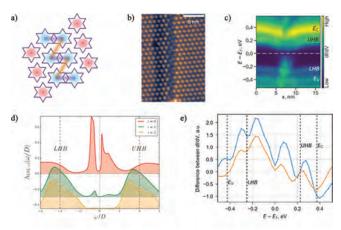


Figure 4: a, b - schematic representation and real-space topography of the domain wall in 1T-TaS2; c - averaged tunnelling spectra evolution across the wall in (b); d - difference between tunnelling spectra inside and outside the domain wall (blue and orange curves correspond to the left and right sides of the domain wall in (b)), emphsizing the existence of the in-gap states; e - DMFT spectral function inside the domain wall showing the collapse of the Mott gap and the formation of two dimerized in-gap levels, consistent with the observed experimental picture in (d).

in the second. To understand the nature of the switching in  $Mo_8O_{23}$  it is important to characterize the phase diagram of the equilibrium state of this less extensively studied compound. Besides two structural transitions close to room temperature it demonstrated that there are apparently uncoupled enigmatic increases in resistivity around ~150 K and below ~30 K, hundreds of degrees below structural transitions. We studied single-particle relaxation dynamics by means of polarized transient reflection spectroscopy and found that besides a small temperature-independent gap present already below first structural transition, additional temperature-dependent depletion of the density of states occurs below ~150 K. The coherent response dynamics as well is very unusual for a CDW compound, with anomalous mode softening at ~200 K, indicating possible competing orders or incipient transitions, as discussed in **Physical Review B**, **99**, **8**, **085101 (2019)**.

#### Theoretical studies on the nanoscale

We developed the theory of magnetoresistance in organic semiconductors, which is based on Pauli blocking principles. The kinetic equations for polaron hopping in organics were derived. At low applied voltages these equations are equivalent to the generalized Miller-Abrahams resistor network and include the effect of spin relaxation on the system's resistivity. The magnetoresistance increases with the applied voltage in agreement with the experiment. (Phys. Rev. B 97, 094201 (2018).)

We developed the model of the phase transition of the second order for the Coulomb frustrated 2D charged system. We found that in such a system, the appearance of the phase-separated state is possible and the transition becomes efficiently first order. As a result, the system undergoes a series of phase transitions when the temperature decreases. First, the system moves from the homogeneous state with a zero order parameter to the phase-separated state with two phases in one of which the order parameter is zero and, in the other, it is non-zero. Then a first-order transition occurs to another phase-separated state, in which both phases have different and non-zero values of the order parameter. Only a further decrease of the temperature leads to a transition to a homogeneous ordered state. (Phys. Rev. B 97, 094415 (2018).)

Based on first-principles calculations and theoretical considerations we show that all-oxide heterostructures incorporating a ferroelectric constituent, such as  $BaTiO_3/La_2CuO_4$ , allow the creation of 2DEG. We predict the possibility of a high-temperature quasi-two-dimensional superconducting state in such 2DEG. The 2DEG could be switchable between superconducting and conducting states by ferroelectric polarization reversal. We also demonstrate that such structures are simple to prepare. The proposed concept of a ferroelectrically controlled interface superconductivity offers the possibility to design novel electronic devices. (Phys. Rev. B 98, 094522 (2018).)

We propose a new and universally applicable viewpoint on charge ordering in triangular lattices based on the sparse ordering of polarons subject to (only) screened Coulomb interactions. Using a charged lattice gas model, our parallel tempering Monte Carlo simulations find stable, regularly ordered polaronic crystals at certain magic filling fractions  $f_m = 1/3, 1/4, 1/9, 1/13, 1/16$  which are observed as commensurate charge density waves in different materials.

In large regions of doping between  $f_m$ , an apparently infinite number of configurationally near-degenerate states result in an amorphous state, which is stable down to very low temperatures. The effective degeneracy of configurational states subject to quantum fluctuations can lead to a quantum charge liquid at low temperatures, analogous to the canonical quantum spin liquid. (arXiv:1901.02232)

#### Nanomaterials

Molybdenum nitrides and carbides that are used as hard coatings or corrosion and abrasion resistant layers, are in general considered as having good chemical resistance. We find, however, that molybdenum nitrides and carbides promptly react with lead nitrate in water at room temperature, resulting in the formation of lead molybdates. The performed one-step reaction, which is very fast and requires no additional reagents, clearly shows the chemical reactivity of molybdenum nitrides and opens a new use for molybdenum nitrides as starting materials in a variety of chemical reactions. At the same time, the demonstrated reaction presents a new method for the synthesis of lead molybdate nanoparticles or hybrid materials using molybdenum nitride or carbide nanowires nanowires. We have protected the disclosure with a Slovenian patent application P-201700312 and continue to protect the invention with the procedure of an international patent application. We discovered a straightforward technique to synthesize molybdenum quasi-one-dimensional structures (microwires, nanowires, nanobelts) from bundles of MoSI NWs as precursor templates. The structural transformations occur when MoSI NWs are annealed in an Ar/ H, mixture, leading to the formation of pure metal with similar structures as initial morphologies. The obtained large-diameter (>15 nm) molybdenum nanowires are highly porous, while small diameters (<7 nm) are made of solid nanocrystalline grains. The method also enables the formation of a foil composed of oriented molybdenum nanowires using a MoSI nanowire foil as the starting material. We have protected the disclosure with European patent EP 2723524 (2018).

#### Soft Matter

We investigated the mechanical tunability of the optical diffraction properties of holographic gratings recorded in a monodomain side-chain liquid-crystalline elastomer (LCE). At temperatures, far below the nematicparanematic phase transition, straining affects mainly the diffraction pattern, while the diffraction efficiency remains almost constant. In contrast, at temperatures close to the nematic-paranematic phase transition, the diffraction efficiency is also significantly affected. The observations were analysed in the framework of the phenomenological model that takes into account strong coupling between the nematic orientational order of the mesogenic groups and the internal strain, which is a characteristic property of LCEs. The results were published in *Appl. Sci.* 8, 1330 (2018).

In cooperation with Nankai University in China we continued investigations of liquid-crystal alignment at the interface with thin polymeric walls that are oriented in the direction perpendicular to *the glass substrates. The walls are fabricated by 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

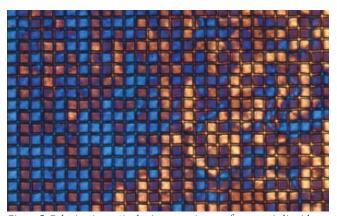


Figure 5: Polarization optical microscopy image of a nematic liquid crystal trapped in a periodic assembly of polymeric square wells with a size of  $10 \times 10 \,\mu\text{m}^2$ .

possibilities for applications in liquid crystalline optical modulators and spatial light filters, microfluidic units based on liquid crystals, etc. The EU patent on this alignment method was granted in 2018 *EP2977815 (B1)*. The results of our investigation of optical-mode coupling in cholesteric liquid crystals separated by periodic polymeric layers were published in *Polymers* 10, 805-1-9 (2018). Part of the collaborative research is also focused on investiga-

tions of multi-stable liquid-crystal configurations in periodic assemblies of square wells prepared by the above-described direct-laser-writing method. We investigated the electric- and magnetic-field-induced switching between different configurations.

Another part of the cooperative research with Nankai University in China was focused on the investigation of calcium-waves-based communication processes between microglial cells. In this study the cells were grown

on special platforms with pre-determined spatial patterns and intercellular signal transmission was analysed as a function of the stimulation site on the central cell and as a function of the distance between the central cell and the neighbouring cells. The results of this work were reported in *ACS Appl. Mater. Interfaces* 10, 2937 (2018). In 2018 we extended our cooperation to investigations of the mechanical properties of biological cells exposed to a liquid flow in patterned microfluidic assemblies. The first results of those investigations were recently submitted for publication in a journal covering the field of microfluidics.

We investigated the mechanisms of molecular recognition of lipophilic derivatives of guanosine in Langmuir films at the air-water interface. The research was based on measurements of modifications in the surface pressure

of the film depending on its irradiation with light of two different wavelengths. In this analysis, photosensitive guanosine derivatives were used as sensors for the formation of base pairs. We also developed a theoretical model for describing the influence of illumination on the molecular organization in the film. At the end of the year, we prepared an article on the above results, which was sent for publication in a journal covering the field of interfaces and thin films.

In collaboration with the Department of Biotechnology (B3), we have recently started working on plasmid DNA containing extended G4C2 repeats. An increased number of G4C2 repeats within the C9orf72 gene is the most common mutation associated with neurological disorders amyotrophic lateral sclerosis and frontotemporal dementia. We used atomic force microscopy to locate and visualize the G4C2 repeat regions based on the formation of G-quadruplex structures inside the plasmid DNA.

In cooperation with University of Vienna we continued investigations of synthetic magneto-active periodic media that might be suitable for application in magnetically tuneable neutron-optical devices. With Monte-Carlo simulations we analysed the neutron transmission through nanocomposite materials. The results were published in *Nulc. Instrum. Methods Phys. Res. A* 916, 154 (2019). We developed a new method for the detection of DNA base pairing in nucleoside thin films. The method is based on the use of photosensitive guanosine derivatives.

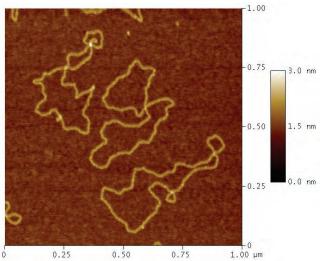


Figure 6: Plasmid DNA molecules adsorbed onto atomically flat mica substrates.

We continued investigations of the surface properties of magneto-active elastomers. The samples were prepared at the East-Bavarian Technical High School (OTH) in Regensburg. Modifications of the surface roughness as a function of applied external magnetic field were determined. We also investigated the effect of magnetic field on the contact angle of sessile water droplets deposited on the material surface. We found that the observed phenomenon of the magnetic-field-dependent contact angle originates predominantly from the field-induced protrusion of carbonyl iron microparticles from the surface layer, while field-induced roughness modifications are practically unimportant. The work was reported in *J. App. Polym. Sci.* 135, 46221 (2018).

In cooperation with the University of Maribor we concluded investigations of the kinetics of water sorption into textile fibers designed for the fabrication of medical textiles. We found that in the case of polyester fibers the sorption speed obtained from optical video-microscopy-based analysis focused on single fibers and the sorption speed obtained from the standard measurement method involving macroscale samples are very similar. The results were published in *Mater. Res. Express* 5, 01531 (2018).

Successful realization of ferromagnetic nematic liquid crystals has opened up the possibility to experimentally study a completely new set of fundamental physical phenomena. The hydrodynamics of such a complex fluid with multiple order parameters is governed by a set of dynamic equations with many material constants, of which only

#### We studied the transition from a uniaxial to a novel nematic phase characterized by a periodic splay modulation of the director and named the new phase a splay nematic phase.

some are easily measurable. In collaboration with theoretical physicists from the Department of Mathematics and Physics, University in Ljubljana, University of Bayreuth and MPI for Polymer Research, Mainz, Germany, we investigated the dynamics of the magneto-optic response experimentally and theoretically and found that it is significantly affected by the dissipative dynamic cross-coupling between the nematic and magnetic order parameters (*Phys. Rev. E* 97, 012701 (2018)). We also conducted a detailed

investigation of some aspects of the static response and the complex dynamics of ferromagnetic liquid crystals under the application of an external magnetic field. The dynamics of the director were measured by optical methods and analyzed in terms of a theoretical macroscopic model. We examined the dependency of dissipative dynamic cross-coupling coefficient on material parameters and the saturation magnetization and the liquid-crystal host. Despite the complexity of the system, the theoretical description allows for a proper interpretation of the results and is connected to several microscopic aspects of the colloidal suspension (*Soft Matter 14*, 7180-7189 (2018)).

In collaboration with researchers from University of York, UK, we studied a recently designed nematic phase, which appears in materials made of polar wedge-shaped molecules. We discovered that the average molecular orientation in the new phase organizes in a manner that resembles a modulated array of Japanese fans. The modulated structure is biaxial and antiferroelectric. The described splay nematic phase is a major step forward towards the realization of an often-speculated polar nematic phase, which could lead to materials with optical and electrical behaviors desired for a wide range of applications. (*Phys. Rev.* X 8, 041025 (2018)).

#### 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 the nonlinear optical conversion of existing lasers into short-wavelength spectral regions where lasers are not yet available.

AIN is a wide-bandgap semiconductor with emerging applications also in nonlinear and quantum optics. Quasi phase matching allows us to use the largest nonlinear optic coefficient in the UV and promises a high conversion efficiency for second harmonic generation. We study AlGaN waveguides in various geometries that allow for phase matched second harmonic generation and therefore give high efficiency. We study phase matching in multimode waveguides and specially prepared waveguides with an alternating sign of the nonlinear coefficient that allows quasi phase matching. The results were reported in *Appl. Sci.* 8, 1218 (2018). AlGaN grown by metalorganic chemical vapor deposition (MOCVD) has 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. New applications in quantum optics are envisioned by writing qubits in nitrogen vacancies.

In collaboration with company Rainbow Photonics and Zurich University of Applied Sciences (Institute of Computational Physics) from Switzerland we study the use of organic electro-optic crystals for the detection of broadband THz radiation (1 to 20 THz).

#### **Biomedical optics**

We have continued with development of novel biomedical applications based on photo-thermal radiometry (i.e., time-resolved measurements of laser-induced infrared emission) and diffuse reflectance spectroscopy (DRS).

By combining these experimental techniques with a dedicated numerical model of light transport in strongly scattering biological tissues, we have developed a unique approach for noninvasive characterization of human skin in vivo in terms of several physiologically relevant parameters (e.g., the contents and oxygen saturation levels of dermal blood). The assessed epidermal thickness values were confirmed by co-registration with multiphoton microscopy, which provides a vertical sectioning capability based on two-photon excited fluorescence (TPEF) and second-harmonic generation (SHG) in different constituents of the skin. (Collaboration with Beckman Laser Institute and Medical Clinic, University of California at Irvine) (*Appl. Opt.* vol. 57, D117, 2018)

The described methodology was tested in several experiments, e.g., involving manipulation of perypheral blood circulation by a pressure cuff. The same approach was also applied to the characterization of hemodynamics in volunteers with incidentally obtained bruises (hematomas). An improved understanding of bruise healing dynamics and derived methodology could enable more accurate determination of the time of injury in forensic investigations.

Our three-dimensional model of light transport in spatially heterogeneous optically scattering structures (Monte Carlo) was used in the analysis of interactions between intense laser pulses and blood vessels with and without the addition of innovative nanostructures, engineered from animal erythrocytes and containing indocyanine green, an FDA approved infrared absorbing dye. The model geometry was based on a blood vessel plexus in a volunteer with a port-wine-stain lesion, characterized using optical coherence tomography. (Collaboration with University of California at Riverside and Beckman Laser Institute and Medical Clinic, University of California at Irvine, USA). (J. Biomed. Opt., vol. 23, 121616, 2018)

We have participated in the research of inorganic nanoparticles that exhibit up-conversion fluorescence (UCF; e.g., Yb<sup>3+</sup>, Tm<sup>3+</sup>:NaYF<sub>4</sub>). Such nanoparticles have great potential for diagnostic imaging in medicine and new approaches for cell-specific therapy. We have investigated nanocomposites with an anisotropic magneto-optic response, based on the nanoparticle UCF and the anisotropic magnetic properties of barium hexaferrite platelets. (Collaboration with Department for Materials Synthesis, IJS).

We have performed an experimental study of hyperthermic lipolysis

using an Nd:YAG laser (wavelength 1064 nm) and forced-air cooling in a porcine model ex vivo. The results show that varying the irradiation power density and duration, as well as the cooling power, enables versatile control over the amplitude and shape of the subsurface temperature distribution. The developed numerical model and improved understanding provide a good basis for a further improvement of laser lipolysis treatment. (Collaboration with Fotona, d.o.o., and Faculty of Mechanical Engineering, University of Ljubljana) (*Lasers Surg. Med.*, vol. 50, 125, 2018)

#### Microfluidics

In close collaboration with the Laboratory for Experimental Soft Matter at the Faculty of Mathematics and Physics and Condensed Matter Physics Department, we created artificial microfluidic swimmers. The micro-swimmers, which swim in the low Reynolds number regime, must perform non-reciprocal movements in order to propel through the fluid. Although there are several ways to achieve this in the laboratory, we discovered a new mechanism for

swimming. The swimmers were composed of superparamagnetic microspheres. By using alternating external magnetic field, the force between the individual swimmer components changed, and consequently the hydrodynamic drag within the swimming cycle. This enabled the introduction of asymmetry into the otherwise periodic movement and resulted in the required non-reciprocity. We created two types of swimmers and have

We created two new types of artificial magnetic microswimmers that can move through complex microfluidic channels.

shown that such swimmers can move in all directions in the sample plane, even through complex microfluidic channels. We studied their motion as a function of the actuation parameters and compared the obtained results with a numerical model. Simulations were the key to understanding the swimming mechanism and gave important additional information that we were not able to obtain from the experiment (Soft Matter, vol. 14, 3415-3422, 2018).

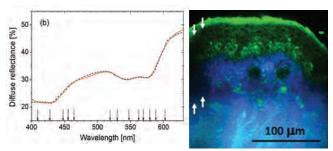


Figure 7: DRS spectrum as measured in the forearm of a volunteer with healthy skin (orange line, left) and best-fitting prediction of our numerical model (dashed). Cross-sectional image of the same skin site obtained by multi-photon microscopy (right).

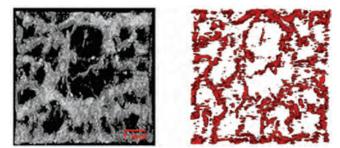


Figure 8: Three-dimensional rendering of a human port-wine-stain (PWS) lesion obtained by optical coherence tomography (left), and calculated damage profiles to the same blood vessel plexus with laser irradiation at 577 nm and 6 J/cm<sup>2</sup> in moderately pigmented skin (right).

We have participated in the research of two types of nanostructures with great potential for applications in biomedical imaging and therapy: lanthanide-doped fluoride nanocrystals featuring up-conversion fluorescence, and nanostructures derived from animal erythrocytes containing the infrared-absorbing dye ICG. Another field of research was the study of particle motion in the side chambers of microfluidic channels. We experimentally confirmed the appearance of secondary flow in side chambers and numerically simulated the possible use as sensors. We analyzed in detail the motion of the particles in the stream and confirmed the correlation between the particle motion and the flow velocity in the main channel. The work was carried out as a final master's thesis entitled *Microfluidic flow sensor based on the observation of particle motion in side chambers*.

We also developed a new method for measuring the Soret coefficient, which is defined as the ratio between the thermodiffusion and the diffusion coefficients of a particle. The method is based on observations of a single particle in an aqueous environment. Once a constant temperature gradient in the sample is established, the Soret coefficient is determined from the velocity of the moving particles. The work was done as a master's thesis entitled *Measurement of the Soret coefficient on individual microparticles*.

Microfluidic research was expanded to studying liquid crystals in microfluidic circuits. In cooperation with the Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, we studied the appearance of electroconvective vortices in microfluidics using nematic liquid crystals. By combining microfluidics with laser light pulses that locally heat and reorient the liquid crystal, we observed the nucleation, manipulation and stabilization of orientational states and domains. This work was carried out in cooperation with the Institute of Biophysics at the Faculty of Medicine. We started investigating the dynamic behaviour of ferrofluids in microfluidic circuits and the research is still ongoing.

#### Some outstanding publications in the past year

- Ravnik, Jan, Vaskivskyi, Igor, Mertelj, Tomaž, Mihailović, Dragan. Real-time observation of the coherent transition to a metastable emergent state in 1T-TaS[subg2. *Physical review. B*, ISSN 2469-9950, 2018, vol. 97, no. 7, str. 075304-1-075304-7, doi: 10.1103/PhysRevB.97.075304. [COBISS.SI-ID 31265831]
- Naseska, Mimoza, Pogrebna, Anna, Cao, G., Xu, Z. A., Mihailović, Dragan, Mertelj, Tomaž. Ultrafast destruction and recovery of the spin density wave order in iron-based pnictides : a multipulse optical study. *Physical review. B*, ISSN 2469-9950, 2018, vol. 98, no. 3, str. 035148-1-035148-13, doi: 10.1103/ PhysRevB.98.035148. [COBISS.SI-ID 32118055]
- Stojchevska, Ljupka, Šutar, Petra, Goreshnik, Evgeny A., Mihailović, Dragan, Mertelj, Tomaž. Stability of the light-induced hidden charge density wave state within the phase diagram of 1T-TaS<sub>2-x</sub>Sex. *Physical review. B*, ISSN 2469-9950, 2018, vol. 98, no. 19, str. 195121-1-195121-6, doi: 10.1103/PhysRevB.98.195121. [COBISS.SI-ID 31991591]
- Madan, Ivan, Buh, Jože, Baranov, Vladimir V., Kabanov, Viktor V., Mrzel, Aleš, Mihailović, Dragan. Nonequilibrium optical control of dynamical states in superconducting nanowire circuits. *Science advances*, ISSN 2375-2548, [in press] 2018, 7 str., doi: 10.1126/sciadv.aa00043. [COBISS.SI-ID 31329831]
- Shumilin, A. V., Kabanov, Viktor V., Dediu, V. I. Magnetoresistance in organic semiconductors : including pair correlations in the kinetic equations for hopping transport. *Physical review. B*, ISSN 2469-9950, 2018, vol. 97, no. 9, str. 094201-1-094201-9, doi: 10.1103/PhysRevB.97.094201. [COBISS.SI-ID 31240487]
- Mamin, R. F., Shaposhnikova, T. S., Kabanov, Viktor V. Phase separation and second-order phase transition in the phenomenological model for a Coulomb-frustrated two-dimensional system. *Physical review. B*, ISSN 2469-9950, 2018, vol. 97, no. 9, str. 094415-1-094415-7, doi: 10.1103/PhysRevB.97.094415. [COBISS. SI-ID 31278631]
- Kabanov, Viktor V., Piyanzina, I. I., Tayurskii, D. A., Mamin, R. F. Towards high-temperature quasi-twodimensional superconductivity. *Physical review. B*, ISSN 2469-9950, 2018, no. 98, no. 9, str. 094522-1-094522-5, doi: 10.1103/PhysRevB.98.094522. [COBISS.SI-ID 31760167]
- Joshua M. Burns, Wangcun Jia, J. Stuart Nelson, Boris Majaron, Bahman Anvari. Photothermal treatment of port-wine stains using erythrocyte-derived particles doped with indocyanine green: a theoretical study. *Journal of biomedical optics*, vol. 23, no. 12, str. 121616-1-10, 2018, doi: 10.1117/1.JBO.23.12.121616. [COBISS.SI-ID 31915559]
- Matija Milanič, Blaž Tašič Muc, Matija Jezeršek, Matjaž Lukač. Experimental and numerical assessment of hyperthermic laser lipolysis with 1,064 nm Nd: YAG laser on a porcine fatty tissue model. *Lasers in* surgery and medicine, vol. 50, iss. 2, str. 125-136, 2018, doi: 10.1002/lsm.22743. [COBISS.SI-ID 3128420]
- Vilfan, Mojca, Osterman, Natan, Vilfan, Andrej. Magnetically driven omnidirectional artificial microswimmers. Soft matter, vol. 14, no. 17, str. 3415-3422, 2018, doi: 10.1039/C8SM00230D. [COBISS.SI-ID 31360551]
- Xing, Fulin, Zhang, Ping, Jiang, Pengchong, Chen, Ziyuan, Yang, Jianyu, Hu, Fen, Drevenšek Olenik, Irena, Zhang, Xinzheng, Pan, Leiting, Xu, Jingjun. Spatiotemporal characteristics of intercellular calcium wave communication in micropatterned assemblies of single cells. *ACS applied materials & interfaces*, vol. 10, iss. 3, str. 2937-2945, 2018, doi: 10.1021/acsami.7b15759. [COBISS.SI-ID 3162724]

- 12. Mertelj, Alenka, Cmok, Luka, Sebastián Ugarteche, Nerea, Mandle, Richard J., Parker, Rachel R., Whitwood, Adrian C., Goodby, J. W., Čopič, Martin. Splay nematic phase. *Physical review. X*, vol. 8, no. 4, str. 041025-1-041025-12, 2018, doi: 10.1103/PhysRevX.8.041025. [COBISS.SI-ID 31856167]
- 13. Lisjak, Darja, Mertelj, Alenka. Anisotropic magnetic nanoparticles : a review of their properties, syntheses and potential applications. *Progress in Materials Science*, vol. 95, str. 286-328, 2018, doi: 10.1016/j. pmatsci.2018.03.003. [COBISS.SI-ID31275559]
- Sebastián Ugarteche, Nerea, Osterman, Natan, Lisjak, Darja, Čopič, Martin, Mertelj, Alenka. Director reorientation dynamics of ferromagnetic nematic liquid crystals. *Soft matter*, vol. 14, no. 35, str. 7180-7189, 2018, doi: 10.1039/C8SM01377B. [COBISS.SI-ID 31669287]

#### Awards and Appointments

- 1. Mimoza Naseska: Best poster award, International Workshop Quantum Complex Matter (QCM 2018) and Frontiers Condensed Matter Physics (FCMP), 11–15 June 2018, Rome, Italy, poster "Optical quench and recovery of SDW state SeFe,As, and EuFe,As,"
- 2. Mimoza Naseska: Best poster award, 2018 Low Energy Electrodynamics of Solids (LEES) conference, 24–29 June 2018, Portonovo, Italy, poster "Optical quench and recovery of SDW state SeFe<sub>2</sub>As<sub>2</sub> and EuFe<sub>2</sub>As<sub>2</sub>"
- 3. Mimoza Naseska: Faculty Prešeren Award for her work titled "Ultrafast Spin Density Wave dynamics at intense optical pulse excitation", supervisor Assist. Prof. Dr Tomaž Mertelj

#### Organization of conferences, congresses and meetings

- 1. Information day for the vertical value chain Advanced sensors and Horizontal Nanotechnology Network, Velenje, Slovenija, 29 November 2018
- 2. Nonequilibrium Quantum Dynamics and Relaxation Phenomena in Many Body Systems, Krvavec, Slovenia, 16-19 December 2018

#### Patent granted

 Xinzheng 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, EP2977815 (B1, European Patent Office, 05. 09. 2018.

## INTERNATIONAL PROJECTS

- Kimberly-Clark Development of LCD Shutter in the Year 2018 Dr. Andrej Petelin Kimberly-Clark
- 7FP TRAJECTORY, Coherent Trajectories through Symmetry Breaking Transitions Prof. Dragan Dragoljub Mihailović
- European Commission
   COST CM1403: The European Upconversion Network From the Design of Photon-Upconverting Nanomaterials to Biomedical Applications Prof. Boris Majaron
  - COST Office
- COST CA16101; MULTI-modal Imaging of FOREnsic SciEnce Evidence tools for Forensic Science
- Prof. Boris Majaron COST Office
- COST CA16218; Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies
- Prof. Viktor Kabanov COST Office
- COST MP1305; Flowing Matter Dr. Mojca Vilfan COST Office
- COST CA17123; MAGNETOFON; Ultrafast Opto-Magneto-Electronics for Non-Dissipative Information Technology
- Prof. Dragan Dragoljub Mihailović COST Association AISBL
- COST CA17140 Nano2Clinic; Cancer Nanomedicine From the Bench to the Bedside Prof. Boris Majaron
- Cost Association Aisbl
- H2020 MagNem; Hydrodynamics of Ferromagnetic Nematic Liquid Crystals Asst. Prof. Alenka Mertelj European Commission
- H2020 Umem4QC; Ultrafast Charge Density Wave Memory or Quantum Computing Prof. Dragan Dragoljub Mihailović European Reasearch Council Executive Agency
- 11. Micro-Patterned Liquid Crystalline Structures for Application in Microfluidic Devices Prof. Irena Drevenšek Olenik
- Slovenian Research Agency 12. Magnetically Reconfigurable Elastomeric Optical Surfaces Prof. Dragan Dragoljub Mihailović
- Slovenian Research Agency 13. The Development of a Nonde
- 13. The Development of a Nondestructive Analytical Method for the Screening of Upconverting Nanoparticles Surface Properties Based on Optical Characterization Prof. Boris Majaron Slovenian Research Agency
- Design and Synthesis of Chemically Stable Luminescent Core-Shell Upconverting Nanoparticles for Bioimaging

## VISITORS FROM ABROAD

- Dr Yelyzaveta Chernolevska, Faculty of Physics of Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, 12–15 March 2018
- Prof. Roman Sobolewski, University of Rochester, Rochester, New York, US, 15–18 March 2018
- Prof. Duncan Haldane, Princeton University, Princeton, New Jersey, US, 18– 24 March 2018
- Dr Andrei Leontev, Zavoisky Physical-Technical Inst. of FIC Kazan SC RAS, Kazan, Russia, 9–14 Aril 2018
- Dr Rinat F. Mamin, Zavoisky Physical-Technical Inst. of FIC Kazan SC RAS, Kazan, Russia, 11–22 April 2018
- 6. Prof. Yasunori Toda, Hokkaido University, Hokkaido, Japan, 31 May to 2 June 2018
- 7. Prof. Migaku Oda, Hokkaido University, Hokkaido, Japan, 31 May to 2 June 2018
- 8. Dr Hiroyoshi Nobukane, Hokkaido University, Hokkaido, Japan, 31 May to 2 June 2018
- 9. Koichi Nakagawa, Hokkaido University, Hokkaido, Japan, 31 May to 2 June 2018
- 10. Vitomir Sever, Institut National des Sciences Appliquées (INSA), Lyon, France, 1 June to 31 August 2018
- Wolfgang Kettl, Ostbayerische Technische Hochschule Regensburg, Regensburg, Germany, 13–29 June 2018
- Alexander Brunhuber, Ostbayerische Technische Hochschule Regensburg, Regensburg, Germany, 13–29 June 2018
- 13. Maria D'Antuono, Department of Physics of the University of Naples and CNR-SPIN, Naples, Italy, 27 June-20 July 2018
- Dr Rinat F. Mamin, Zavoisky Physical-Technical Inst. of FIC Kazan SC RAS, Kazan, Russia, 4 July–4 August 2018

Prof. Boris Majaron Slovenian Research Agency

- Liquid Crystalline Properties of Guanosine-Rich DNA and RNA Oligonucleotides Prof. Irena Drevenšek Olenik
- Slovenian Research AgencyPhoto-Stimulated Phenomena and Dynamical States in the Vicinity of the Phase Transition

Prof. Viktor Kabanov Slovenian Research Agency

### RESEARCH PROGRAMS

- 1. Medical physics
- Dr. Matija Milanič 2. Light and Matter
- Light and Matter Prof. Irena Drevenšek Olenik
- Dynamics of complex nano-systems Prof. Dragan Dragoljub Mihailović
- **R & D GRANTS AND CONTRACTS**
- 1. Femtosecond time-resolved scanning tunneling electron microscopy of complex materials
- Prof. Dragan Dragoljub Mihailović
   Electrically tunable ferromagnetic liquids
- Asst. Prof. Alenka Mertelj
- Probing spin states near the surface of quantum spin materials Petra Šutar
- Phase transitions in systems of nucleotide repeat expansions associated with neurodegenerative diseases Prof. Irena Drevenšek Olenik
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Dragan Dragoljub Mihailović
- Ministry of Economic Development and Technology 6. Development of gradual optical shutter - OPTIGRAD
- Dr. Luka Cmok Ministry of Education, Science and Sport
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Dragan Dragoljub Mihailović
- Ministry of Economic Development and Technology 8. Microfluidic Systems Based on Anisotropic Soft Matter Prof. Irena Drevenšek Olenik
- ZRC SAZU
   Advancing Charge Density Wave Memory Device Science and Technology Prof. Dragan Dragoljub Mihailović

NFFA.eu

- Yevhenii Vaskivskyi, Taras Shevchenko National University Kyiv, Kyiv, Ukraine, 4–30 August 2018
- Dr Luca Sapienza, Department of Physics & Astronomy, University of Southampton, Southampton, UK, 29 July to 3 August 2018
- Camila Honorato Rios, University of Luxembourg, Luxembourg, Luxembourg, 15–20 July 2018
- Dr Yelyzaveta Chernolevska, Taras Shevchenko National University Kyiv, Kyiv, Ukraine, 31. August to 3 October 2018
- Dr Jon Wulff Petersen, Plougmann Vingtoft tto, Copenhagen, Denmark, 28– 29 August 2018
- Prof. Michele Fabrizio, International School for Advanced Studies SISSA, Trieste, Italy, 4 October 2018
- Song Xiao, TEDA Applied Physics Institute, Nankai University, Tianjin, China, 15–27 October 2018
- Prof. Milena Marinović-Cincović, Nuklearni Institut Vinča, Univerza v Beogradu, Vinča, Serbia, 15–18 October 2018
- Aleksandr Kuntsevich, Laboratory For Condensed Matter Physics Superconductivity and Quantum Materials, National Research University Higher School of Economics of the Russian Academy of Sciences, Moscow, Russia, 18–24 November 2018
- Valerii Prudkogliad, P. N. Lebedev Physical Institute of the Russian Academy of Sciences, Moscow, Russia, 20 November to 2 December 2018
- Dr Ivan Štajduhar, Faculty of Engineering University of Rijeka, Rijeka, Croatia, 3–7 December 2018
- Teo Manojlović, Faculty of Engineering University of Rijeka, Rijeka, Croatia, 3–12 December 2018

### STAFF

#### Researchers

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- 2 Prof. Martin Čopič\*, left 01.11.18
- Prof. Irena Drevenšek Olenik\* 3.
- Prof. Christoph Gadermaier, left 01.08.18 4. Prof. Viktor Kabanov
- 5
- Dr. Matjaž Lukač\* 6.
- Prof. Boris Majaron 7.
- 8 Asst, Prof. Alenka Merteli
- Asst. Prof. Tomaž Mertelj 0
- 10. Prof. Dragan Dragoljub Mihailović, Head
- 11. Dr. Matija Milanič\*
- 12. Dr. Aleš Mrzel
- 13. Asst. Prof. Natan Osterman\*
- 14. Asst. Prof. Lea Spindler\*
- 15. Asst. Prof. Lev Vidmar
- 16. Dr. Mojca Vilfan
- 17. Prof. Marko Zgonik\*
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- 18. Dr. Yelyzaveta Chernolevska
- 19. Dr. Luka Cmok
- 20. Dr. Andrej Petelin
- 21. Dr. Nerea Sebastián Ugarteche 22. Dr. Jure Strle, left 01.04.18

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- 40. Laura Petan, B. Sc., left 01.10.18

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Postgraduates

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# DEPARTMENT OF REACTOR PHYSICS F-8

During the past year we have been working mainly on:

- theoretical, experimental and applied reactor physics
- plasma physics
- neutron transport calculations
- medical physics

In the field of **reactor physics** our activities have been focused on the development of novel methods for research and power reactor analyses.

In the framework of the international collaboration project E-SiCure - Engineering Silicon Carbide for Improved Border and Port Security, which is being carried out under the NATO Science for Peace and Security programme, we have begun the development of neutron detectors based on SiC aimed at the detection of fissile material. We produced several SiC detector prototypes with different converter layers made of 10B and 6Li that convert neutrons into ions (4He and 3H). The detectors' performance was tested in a dry chamber of the JSI TRIGA reactor and the responses of the individual detectors were clearly measurable. This is encouraging for future applications.

After several years of research, we updated the Rod Insertion Method for Control Rod Worth Measurement. This was achieved through the simulation of reactor kinetics and analysing the influence on measurement results. The proposed corrections in the post-processing of the neutron flux signal include compensation of the reactivity overshoot, which occurs after the control rods reach the bottom-most position. Overall, a true equivalence has been established between the results of the Rod Insertion Method and those of the reference, time-consuming Boron Dilution Method. Furthermore, we can even distinguish the influence of axial grid straps on the differential worth curve.

In the field of neutron dosimetry, in collaboration with colleagues from CEA – Cadarache and CEA – Saclay, we are studying radiative neutron capture reactions, in themselves predominantly sensitive to the thermal and resonance neutron energy ranges, which would exhibit a sensitivity shift to epithermal neutron energies in conjunction with the appropriate boron-based thermal neutron filters. In neutron dosimetry the epithermal energy range is very poorly covered on account of the small number of radiative capture reactions that have strong resonances at epithermal energies, or threshold reactions with a low energy threshold.

In 2018, we carried out three demanding experimental campaigns on the JSI TRIGA reactor at the IJS during which we tested self-powered neutron detectors, thermocouples and fission chambers under well-characterised conditions. The work was carried out in collaboration with the French institutions CEA in Thermocoax

In this year we have continued to actively participate in the two OCED/ NEA workgroups, namely the International Criticality Safety Benchmark Evaluation Project (ICSBEP) and International Reactor Physics Experiment Evaluation Project (IRPhEP), where we have contributed a new evaluation

of a benchmark experiment with a UO2F2 solution in a spherical geometry. The experiment is crucial for the analysis of reprocessed-fuel criticality measurements. We have taken part in the workgroup meetings and helped with the independent review of foreign benchmark experiment evaluations.

Within the framework of the European CHANDA project, we were involved in the process of improving nuclear data for the fourth-generation reactor concept MYRRHA. For materials and reactions, which significantly influence the uncertainty of integral parameters and have the most room for improvement, a comparison between experimental and evaluated nuclear data was performed.

We continued an international collaboration led by the Swedish organizations Vattenfall, SKB and SSB in the field of spent PWR fuel characterization. In close collaboration with EC-JRC and SCK • CEN we have finished the phase-1 calculations, where the decay heat from PWR fuel assemblies was determined. In the future detailed validation of the decay heat from different fuel assemblies originating from Swedish PWR and BWR reactors will follow. We will focus on sensitivity and uncertainty analyses with the use of different codes and models.



Asst. Prof. Luka Snoj

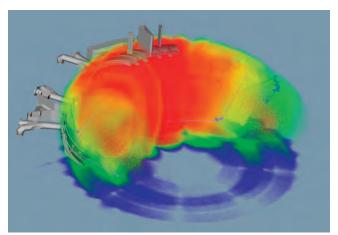


Figure 1: Neutron distribution inside the JET tokamak including a single track out of billions. Calculations are performed on large computer clusters.

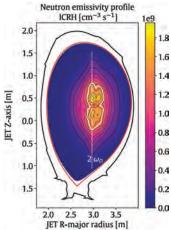


Figure 2: Neutron-emissivity profile computed with the TRANSP code for JET plasma discharge 92436, where both NBI and ICRH systems were used for the plasma heating. The white dotted line denotes the second ion cyclotron resonance layer, while the magnetic axis is denoted with a red cross. The profile is enclosed by the last closed flux surface (red) and JET limiter (black).

Researchers of the Reactor Physics Department provided technical support for the safe operation of the Krško nuclear power plant (NPP) also in 2018. We have independently performed nuclear core design calculations for the fuel cycle 30 and the start-up tests for the new fuel cycle. In addition, the expertise and calculational support for future dry storage of spent nuclear fuel was provided. In the framework of the project financed by the Slovenian Research Agency (sofinanced by the NPP Krško) the McCord code has been developed. The interface will enable the automatic transfer of the fuel characteristics from the CORD-2 system to the MCNP code for an arbitrary operational state. The calibration and verification process of the parameters has been performed. For the Slovenian Nuclear Safety Administration an analysis of the influence of the most important parameters on isotopic composition of the NPP Krško spent fuel and their influence on the intended dry storage of spent fuel has been accomplished.

In the field on neutron-transport simulations for fusion reactors we continued our collaboration with several institutes/laboratories/universities on the analyses of experimental data obtained during the calibration of JET's neutron detectors to 14 MeV neutrons. For this purpose we simulated detector responses to a calibration neutron source (DT neutron generator) and plasma as a source of neutrons inside the reactor. The calibration factors for fission chambers (for time-dependent neutron-yield measurements) and the activation system (for time-integrated neutron-yield measurements) were determined through a combination of measurements and simulations. Computational support was crucial for achieving detector calibration uncertainties lower than the target uncertainty of 10 %. By the end of 2018 most of the calibration procedure was completed. However, the final confirmation will be performed during the DT plasma campaign when the neutron yield measurements from different detectors will be compared. Some additional analyses are still in progress to increase our understanding of the calibration procedure and the reliability of the calculated correction parameters.

In the scope of the European fusion programme (Fusion for Energy–F4E and EUROfusion) we continued our international collaboration in the field of fusion neutronics that started more than 20 years ago. This research includes both experimental and theoretical work. We prepared an evaluation of the benchmark experiment FNG-copper, which was experimentally conducted in 2016-2017. This work is important for the validation of neutron and gamma cross-sections for copper.

Within the EUROfusion project we prepared sensitivity and uncertainty studies of the ASPIS IRON88 benchmark experiment and investigated the use of covariance matrices for angular distributions of scattered neutrons on the uncertainties of integral parameters.

During the international conferences NENE 2018 in Portorož and at the RPSD (Radiation protection and shielding division of the American Nuclear Society) 2018 conference in Santa Fe, USA a workshop was organized on the use of the JSI-developed program package XSUN-2017/SUSD3D, which was attended by a significant number of participants. Researchers from the F8 division performed simulations of the neutron field in various positions inside the JET

tokamak. We collaborated in analyses in support of both future and past experiments. Additionally, we investigated



Figure 3: Visualization of the full 3D model of the JET tokamak used for calculations of streaming experiments. The contour plot shows the neutron flux originating from DT plasma contained in the vacuum vessel simulated using a discrete ordinates deterministic neutron transport code.

the cause for discrepancies in predicted neutron fluxes at lower energies, which were found during calculations with two different models. We prepared a detailed model of the O-LTIS irradiation position, which is located behind the first wall of the JET tokamak. Using the special variance reduction methods for optimisation over the whole neutron energy range we significantly increased the quality of the thermal neutron flux determination and consequently improved preliminary calculations of the reaction rates in materials that will be used in upcoming experiments.

Researchers from the F8 division and RIC collaborated in preparations for the measurements of water activation in the JET tokamak caused by the threshold reaction 16O(n,p)16N. This experiment is important for ITER as it will be a water-cooled machine and the presence of large quantities of the 16N isotope will represent a significant radiological hazard, imposing restrictions on the space near the cooling system outside of the tokamak. At the JET tokamak we performed tests and calibration of the efficiencies of the two scintillator detectors for gamma rays in 2018. They are planned to be used in experiments.

In 2018 we continued with neutronic analyses in support of the DEMO (demonstrational fusion power plant) development process. This work is part of the EUROfusion Engineering Grant and in 2018 included work on different DEMO reactor configurations with the emphasis on the nuclear heating of superconducting magnets due to increased neutron and gamma fields caused by the integration of various systems. Analyses

showed some suitable configurations and useful shielding strategies that will be used in subsequent DEMO designs. These analyses were an important part of the preparation for the DEMO design review conducted by an external panel of experts in May 2019.

In 2018 we continued with an active collaboration within the JET3-NEXP streaming benchmark experiment. We contributed calculations of neutron fluences using Monte Carlo, deterministic and hybrid (Monte Carlo/deterministic) transport codes at several experimental locations inside the JET tokamak building. Calculation results from different transport codes and nuclear data libraries were compared with the experimental results. Experiments were performed using a thermo-luminescent detector and activation foils. This work is being performed in a consortium of international institutions including national laboratories from Slovenia,

Great Britain, Poland, Greece, Italy and the USA.

In 2018 the code package PLANET for detailed calculations of plasma neutron sources has been developed in collaboration with the JET tokamak and PPPL (USA), Uppsala University (Sweden) and UNED (Spain). The code is based on a subroutine written in the programming language Fortran, which is coupled to the advanced Monte Carlo neutron transport code MCNP. The information on the plasma state is computed with the TRANSP plasma transport code, developed at the Princeton Plasma Physics Laboratory. Based on the plasma state description the neutron spectra are computed with the Swedish DRESS code. Obtaining data on the neutronemissivity profile in the JET tokamak, neutron emission vector and energy we can commence the source random sampling procedure and the calculation of a plasma neutron source description. The PLANET code package has been verified and validated using a simplified and detailed JET tokamak computational model. It was found that the neutron yield monitors that are positioned on the outside of the vacuum vessel are relatively insensitive to changes in the neutron source, while activation measurements can be used to record differences in the plasma state and the effects of plasma heating. (ŽIGA)

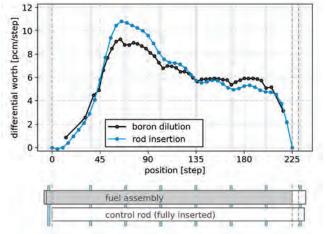


Figure 4: Comparison of differential reactivity worth curves for a control rod bank at Krško NPP. The updated Rod Insertion Method yields practically identical results to the reference, time-consuming Boron Dilution Method. We can also distinguish the influence of axial grid straps.

In the field of **medical physics**, we continued our research in our main areas of interest: modelling, image analysis of positron emission tomography (PET), image-guided cancer treatment and proton therapy. Additionally, we also started with the field of biomedical optics.

We have developed a computational model for simulating the response of pre-clinical tumours to treatment with anti-PD-1 immunotherapy. The model was verified on experimental data from the literature, giving good agreement between the simulations and experimental results. An original scientific article on this model was published in the journal Physics in Medicine and Biology (Valentinuzzi *et al* 2019 *Phys. Med. Biol.* 64 025017). In cooperation with the Department of Experimental Oncology at the Institute of Oncology Ljubljana, we have performed a series of experiments to test the computational model on other types of tumours (besides melanoma). Additionally, the model was extended to simulate a combined treatment with anti-PD-1 immunotherapy and radiotherapy.

In cooperation with the Institute of Oncology Ljubljana, a prospective study with immunotherapy is still underway. Patients with metastatic lung cancer are treated with anti-PD-1 immunotherapy (pembrolizumab) and scanned with diagnostic CT and FDG PET/CT at baseline (before treatment), as well as 1, 4, 10, 16 and 20 months after the treatment's initiation. Currently, we have completed patient accrual with 30 patients being enrolled in the study. By using radiomics analysis of PET/CT images, we will determine if a long-term response of patients can be predicted based on an early metabolic response (after 1 month), which would be significantly faster compared to the current standards (iRECIST).

In the field of proton therapy, a master's thesis entitled "Simulation of the delivered dose in proton therapy in dynamic geometry" was made. In the master's thesis, the process of simulation of the predicted dose distribution was presented for the case of lung-tumour irradiation. Two breathing phases were considered - the inhalation and exhalation phase. The delivered dose distribution was simulated using the Monte Carlo method integrated into the MCNP program.

In the field of biomedical optics, the development of the system for hyperspectral microscopy has been underway. The system's capabilities achieved by now include imaging of samples in a transmission mode in the spectral range between 430 and 730 nm with a spectral resolution of about 2 nm. A conference article about the developed system was presented at the Photonics West 2018 conference.

As always in the recent years, we has a close collaboration with the University of Wisconsin - Madison.

#### Some outstanding publications in the past year

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#### **Organization of Conferences, Congresses and Meetings**

5th Conference of Young Nuclear Experts, "Jožef Stefan" Institute, Ljubljana, Slovenia, 26. 2. 2018

## INTERNATIONAL PROJECTS

- 1 7FP - CHANDA; solving CHAllenges in Nuclear Data Prof. Ivan Aleksander Kodeli European Commission
- F4E-FPA-395-02; Gas Production Experiment and TBM Nuclear Instrumentation 2 Prof. Ivan Aleksander Kodeli
- The European Joint Undertaking For The Development
- Benchmarks of Computational Tools against Experimental Data on Fuel Burnup and 3. Material Activation for Utilization, Operation and Safety Analysis of Research Reactors; Activation Rate Benchmark at the JSI TRIGA Mark-II Reactor Dr. Vladimir Radulović
  - IAEA International Atomic Energy Agency
- 4. E-SiCure - Engineering Silicon Carbide for Enhanced Border and Ports Security Prof. Luka Snoj
- Nato North Atlantic Treaty Organisation
- Kinetic Approach to Modelling and Measurements in SOL of Tokamak; Network of Small and Medium Size Magnetic Confinement Fusion Devices for Fusion Research Dr. Jernej Kovačič
- IAEA International Atomic Energy Agency
- 6 H2020 EUROfusion - Research Unit - Administration and Services RU - FU Prof. Luka Snoj
- European Commission
- 7. H2020-EUROfusion-Plasma Facing Components-1-IPH-FU, EUROFUSION Dr. Jernej Kovačič
- European Commission H2020-EUROfusion; Exploatation of DT Operation for ITER-JET3-FU Prof. Luka Snoj
- European Commission
- H2020 EUROfusion Education-ED-FU Prof. Luka Snoi
- European Commission
- 10. H2020 EUROfusion JET Campaigns-JET1-FU Dr. Žiga Štancar
- European Commission 11. H2020 EUROfusion - Medium Size Tokamak Campaigns-MST1-FU
- Dr. Jernej Kovačič European Commission
- 12. H2020 EUROfusion JET Enhancements-JET4-FU, EUROFUSION Prof. Igor Lengar
- European Commission 13. H2020 EUROfusion - PMI-PPPT-2-FU: Nuclear data
- Prof. Ivan Aleksander Kodeli European Commission
- 14. H2020 EUROfusion Engineering Grants: Fusion Plant Nuclear Analyst The modelling of the proposed DEMO component designs, testing their performance under reactor conditions and development of new design solutions Dr. Aliaž Čufar
- European Commission
- 15. 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
- 16. Combined Use of Monte Carlo and Deterministic Particle Transport Tools for Fusion Shielding Benchmark Neutronics Studies Prof. Ivan Aleksander Kodeli Slovenian Research Agency
- 17. Multiphysics Validation of High Fidelity Modelling and Simulation for Nuclear

- Applications Prof. Luka Snoi
- Slovenian Research Agency
- 18. Accelerating Neutronics Analyses for Fusion and Fission Applications Using the ADVANTG Code
  - Prof. Luka Snoj
  - Slovenian Research Agency
- 19. Generation of a Plasma Neutron Source through the Coupling of Plasma Simulation Programs and Monte Carlo Neutron Transport Codes Prof. Igor Lengar
- Slovenian Research Agency
- 20. Experimental and Numerical Research in Support of Development of Plasma Potential Probes
  - Dr. Jernej Kovačič
  - Slovenian Research Agency
- 21. Multiphysics Validation of High Fidelity Modelling and Simulation for Nuclear Applications
- Dr. Vladimir Radulović
- Slovenian Research Agency
- 22. Use of Shielding Benchmarks for Nuclear Data Validation and Improvement Prof. Ivan Aleksander Kodeli Slovenian Research Agency
- 23. Eksperimental validation of the gamma flux simulation scheme and measurment techniques by TLD, OSLD and ionization chamber in the mixed neutron-photon high dose rate environment of the JSI TRIGA reactor Prof. Luka Snoj
- Slovenian Research Agency 24. 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
- 25. Consequences of electron emission from hot plasma-facing components in nuclear fusion reactors
  - Dr. Jernej Kovačič Slovenian Research Agency
- 26. Epithermal neutron flux determination and validation of nuclear cross-sections and through activation measurements employing neutron spectrum filters Prof Andrei Trkov Slovenian Research Agency
- **RESEARCH PROGRAMS**
- 1. Medical physics Prof. Robert Jeraj
- 2. Reactor Physics
- Prof. Luka Snoj

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

- 1. Analysis of nuclear heating in a reactor Prof. Luka Snoj
- Determination of the Am-241 thermal neutron capture cross section by activation measurements at the JSI TRIGA reactor Dr. Gašper Žerovnik
- Development of Computational Tools for the Determination of the Neutron Field in the 3.



Containment of a Pressurized Water Reactor Prof. Andrei Trkov

ICERR Agreement for Receiving Affiliate Staff to CEA as a Designated International 4. Center based on Research Reactors, through its Research Centres of Saclay and Cadarache

Prof. Luka Snoi

- Cea Commissariat A L"energie Atomique Et Aux
- 5. Experimental Testing of Self-Powered Neutron Detector Assembly for CEA DISCOMS Project
  - Dr. Vladimir Radulović
- Cea List Institute, Dept. Of Metrology,
- Experimental Testing of Self-Powered Neutron Detector Assemblies for CEA INFINI 6. Project

## VISITORS FROM ABROAD

- Loic Barbot, Stephane Fourrez, Alternative Energies and Atomic Energy Commission 1 - CEA, DEN / DER / SPEX / LPE, Cadarache, France and Hamid Makil, Thermocoax, Suresnes, France, 15.-19. 1. 2018
- Kamada So, Kato Michio, Nishimura Kazuyo, National Institute of Maritime Port 2. and Aviation Technology, Tokyo, Japan; Ashley Jones and Malcolm Joyce, Lancaster University, Lancaster, United Kingdom; Mathew J. Nancekievill and Watson Simon, University of Manchester, Manchester, United Kingdom; Okumura Keisuke, Japan Atomic Energy Agency (JAEA), Fukushima-ken, Japan; Katakura Junichi, Nagaoka University of Technology, Nagaoka, Japan, 6.-8. 2. 2018
- 3. Prof. Patrick Blaise, Alternative Energies and Atomic Energy Commission - CEA, DEN / DER / SPEX / LPE, Cadarache, France, 20.-22. 2. 2018
- 4 Alexandru-Mihai Bumbac, Robert-Mihai Solomon, "Ovidius" University, Constanța, Romania, 2.-31, 3, 2018
- 5. Chen Linhao, Zhou Yu, Ning Bolun, Gu Min, Sun Xueping, He Xiuping, delegates of the China - Slovenia scientific and technological cooperation committee, Ministry of Science and Technology of the People's Republic of China, Beijing, China, 27. 3. 2018
- Prof. Kord Smith, prof. Benoit Forget, Massachusetts Institute of Technology MIT, Department of Nuclear Science and Engineering, Cambridge, MA, USA, 24.–31. 3. 2018 6
- Dr. Ivana Capan, leader of the international project E-SiCure, Tomislav Brodar, Zoran Ereš, Institut "Rudjer Bošković", Zagreb, Croatia; dr. Željko Pastuović, Adam Sarbut, ANSTO (Australian Nuclear Science and Technology Organization), Lucas Heights, NSW, Australia; dr. Takeshi Ohshima, Yuichi Yamazaki, National Institute for Quantum and Radiological Science and Technology, Chiba, Japan; dr. Jose Courtinho, Universidade de Aveiro, Portugal, 28.-30. 5. 2018
- 8. Dr. Paola Batistoni, ENEA, Frascati, Italy and CCFE, Abingdon, United Kingdom, 20.-23.7.2018
- Thibault Cordier, École National Supérieure d'Informatique pour l'Industrie et
- l'enterprise (ENSIIE), University of Évry Val d'Essonne, Évry, France, 10. 6.-2. 9. 2018 Dr. Pierre Dossantos, International relations, ENSIIE, University of Évry Val d'Essonne, 10. Evry, France, 7. 8. 2018

#### Dr. Vladimir Radulović

Cea List Institute, Dept. Of Metrology,

Experimental Testing of Self-Powered Neutron Detectors for the Thermocoax Company 7. Dr. Vladimir Radulović Thermocoax Sas

### NEW CONTRACT

Characterization of the NPP Krško spent fuel for the purpose of storage in dry containers Asst. Prof. Marjan Kromar

Ministry of the Environment and Spatial Planning

- 11. Aljaž Kolšek, UNED, Madrid, Spain, 10. 8. 2018
- 12. Dr. Christophe Destouches, Gerald Rimpault, CEA, Cadarache, France; Arran Plant, Lancaster University, Lancaster, United Kingdom; Jakub Lüley, Branislav Vrban, Stefan Cerba, Filip Osuský, Slovak University of Technology (STUBA) in Bratislava, Slovakia, 10.-13. 9. 2018
- Thibault Cordier, École National Supérieure d'Informatique pour l'Industrie et 13. l'enterprise (ENSIIE), University of Évry Val d'Essonne, Évry, France, 10.-13. 9. 2018
- 14 Dr. Xiaolei Zheng, dr. Leiming Shang, Institute of Nuclear Energy Safety Technology, Hefei, Anhui, China, 10.-13. 9. 2018
- 15 Tetiana Vorontsova, State Nuclear Regulatory Inspectorate of Ukraine, Kiev, Ukraine; Firdavs Salomov, Nuclear and Radiation Safety Agency of Tajikistan, Dushanbe, Tajikistan, 8. 10.-1. 12. 2018
- 16 Dr. Loic Barbot, Damien Fourmentel, Alternative Energies and Atomic Energy Commission - CEA / DER / SPESO / LDCI, Cadarache, France, 8.-19. 10. 2018
- 17. Dr. Elchin Huseynov, National Nuclear Research Centre, Baku, Azerbaijan, 17.-19.10.2018
- 18. Valerio Mascolino, Virginia Tech, Blacksburgh, Virginia, USA, 13.11. 2018 - 31. 12. 2018 (till 22. 5. 2019)
- Li Dongsheng, Lv Yunfeng, Cai Li, China Nuclear Power Technology Research Institute Co., Ltd., Shenzehen, Guangdong, PR China; Loic Barbot, Alternative Energies and Atomic Energy Commission - CEA, DEN / DER / SPEX / LPE, Cadarache, France; Georges Helleux, Vincent Salou, Laurent Pichon, Thermocoax, Suresnes, France, 19.-30. 11. 2018
- 20. Nicolas Campet, Fargues Stephane Serge, Gaël De Cargouet, Rolls Royce Civil Nuclear Company, Grenoble, France; Hassen Hamrina, Mathieu Trocme, Loic Barbot, Alternative Energies and Atomic Energy Commission - CEA, Cadarache, France, 4.-6. 12. 2018
- Hubert Carcreff, CEA, Saclay and Nicolas Thiollay, CEA, Cadarache, France, 10.-21. 12. 2018

### STAFF

#### Researchers

- Prof. Tomaž Gyergyek\* 1.
- Prof. Robert Jeraj 2
- Prof. Ivan Aleksander Kodeli Asst. Prof. Marjan Kromar 3.
- 5 Prof. Igor Lengar
- Dr. Matija Milanič 6
- Dr. Urban Simončič\*
- Prof. Luka Snoj, Head 8
- 9. Prof. Andrej Trkov Dr. Gašper Žerovnik
- Postdoctoral associates
- 11. Dr. Dušan Čalič\*
- 12. Dr. Aljaž Čufar
- 13. Dr. Jernej Kovačič
- 14. Dr. Vid Merljak
- 15. Dr. Vladimir Radulović

#### Postgraduates

- 16. Klemen Ambrožič, B. Sc.
- 17. Tanja Goričanec, B. Sc.
- 18. Bor Kos, B. Sc.
- 19. Anže Pungerčič, B. Sc. 20. Žiga Štancar, B. Sc.
- 21. Damijan Valentinuzzi, B. Sc.
- 22. Andrej Žohar, B. Sc.
- Technical and administrative staff
- 23. Slavko Slavič, B. Sc.
- 24. Saša Škof, B. Sc.
- 25. Uršula Turšič, B. Sc.
- 26. Bojan Žefran

Note: \* part-time JSI member

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- 13. Aljaž Čufar, Paola Batistoni, Zamir Ghani, Luca Giacomelli, Igor Lengar, Stefano Loreti, Alberto Milocco, Sergey Popovichev, Mario Pillon, Davide Rigamonti, Marica Rebai, Marco Tardocchi, Luka Snoj, and JET Contributors, "Modelling of the neutron production in a mixed beam DT neutron generator", *Fusion engineering and design*, 2018, **136**, B, 1089-1093.
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- 16. Georgi Gorine, G. Pezzullo, Igor Mandić, Anže Jazbec, Luka Snoj, Mar Capeans, Michael Moli, Didier Bouvet, F. Ravotti, J. Sallese, "Ultra high fluence radiation monitoring technology for the future circular collider at CERN", *IEEE transactions on nuclear science*, 2018, 65, 8, 1583 - 1590.
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clinical trials", Journal of applied clinical medical physics, 2018, **19**, 5, 335-346.

- 19. Ivana Capan *et al.* (12 authors), "Double negatively charged carbon vacancy at the h- and k-sites in 4H-SiC: combined Laplace-DLTS and DFT study", *Journal of applied physics*, 2018, **123**, 16, 161597.
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- 21. Matjaž Lukač, Jernej Kukovič, Blaž Tašič Muc, Nejc Lukač, Matija Milanič, "TightSculpting©: a complete minimally invasive body contouring solution. Part I, sculpting with PIANO© technology", *LAHA: journal of the Laser and Health Academy*, 2018, 16-25.
- 22. Matija Milanič, Blaž Tašič Muc, Matija Jezeršek, Matjaž Lukač, "Experimental and numerical assessment of hyperthermic laser lipolysis with 1,064 nm Nd: YAG laser on a porcine fatty tissue model", *Lasers in surgery and medicine*, 2018, **50**, 2, 125-136.
- 23. Ivana Capan, Tomislav Brodar, Takeshi Ohshima, Shin-ichiro Sato, Takahiro Makino, Ž. Pastuović, R. Siegele, Luka Snoj, Vladimir Radulović, JoséCoutinho, V. J. B. Torres, Kamel Demmouche, "Deep level defects in 4H-SiC epitaxial layers", *Materials science forum*, 2018, **924**, 225-228.
- 24. D. A. Brown *et al.* (70 authors), "ENDF/B-VIII.0: The 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data", *Nuclear data sheets*, 2018, 148, 1-142.
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- Michal W. Herman *et al.* (20 authors), "Evaluation of neutron reactions on iron isotopes for CIELO and ENDF/B-VIII.0", *Nuclear data sheets*, 2018, **148**, 214-253.
- 28. R. Capote *et al.* (23 authors), "IAEA CIELO evaluation of neutroninduced reactions on <sup>235</sup>U and <sup>238</sup>U targets", *Nuclear data sheets*, 2018, 148, 254-292.
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#### Monograph

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#### Mentoring

- 1. Aljaž Čufar, Evaluation of methods for power calibration in large tokamaks: doctoral dissertation, Ljubljana, 2018 (mentor Igor Lengar).
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# DEPARTMENT OF EXPERIMENTAL PARTICLE PHYSICS

Departmental research is devoted to experimental studies of elementary particles, to reveal the ultimate building blocks of matter and the nature of the interactions between them. Experiments are carried out within large collaborative programmes at international centres for particle physics, i.e., 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 ultrahigh-energy cosmic rays with the Pierre Auger observatory spread over a surface of 3000 km<sup>2</sup> near Malargue in Argentina.

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

Together with colleagues from the Physics Department of the Faculty of Mathematics and Physics and the Faculty of Electrical Engineering of the University of Ljubljana, and from the Faculty of Chemistry and Chemical

Technology of the University of Maribor, we are performing measurements at CERN and 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, 175 institutions from 38 countries),
- Belle II at the asymmetric electron-positron collider (KEK-B) at KEK (750 researchers, 101 institutions from 22 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.

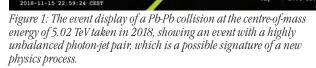
A more detailed report on the 2018 activities follows, focused on the contributions of our researchers:

#### **ATLAS** experiment

In 2015 the upgraded Large Hadron Collider LHC began its operation at CERN and reached a record center-of-mass energy of 13 TeV, which marks the beginning of the "Run 2" of the LHC's operation, which then finished at the end of 2018 with heavy-ion collisions (Pb-Pb) at a centerof-mass energy of 5.02 TeV (Fig.1). In the next two years the detectors and colliders will be upgraded before the next re-start, which also gives us the much-needed time to analyze the data collected so far. In 2015-2018 the LHC 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 in 2015-2018 reached an integrated luminosity of 150 fb<sup>-1</sup> of exceptional data, which led to the most precise Run 2 searches of New Physics beyond the Standard model hitherto achieved. In the analyzed data a considerable number of different theories was excluded and there are some indications for potential new discoveries in the particle physics - however, for confirming or refuting these the full set of recorded data needs to be analyzed. Subsequently, the

will be upgraded before the next re-start, which also gives us the much-needed time to analyze the data collected so far.

In the next two years the detectors and colliders



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next two years will be full of challenges and expectations of pivotal events. In 2018 the ATLAS collaboration published more than 100 scientific papers in the most distinguished scientific journals [1,2], bringing the total number of scientific papers published by the collaboration to 800, with more than a hundred further papers in preparation.

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

Activities at the Belle and Belle II experiments, operating at the electron positron collider KEKB / SuperKEKB in Tsukuba, Japan, continued. The aim of the experiments, belonging to the group of intensity frontier efforts, is

## In 2018 the Belle II detector successfully underwent commissioning and recorded the first data in $e^+e^-$ collisions.

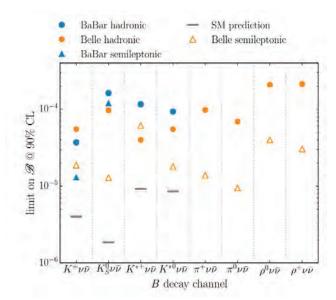


Figure 2: Existing upper limits on  $B \rightarrow hvv$  decays, for several species of light hadron h. Results marked with triangle are from a recent Belle measurement.

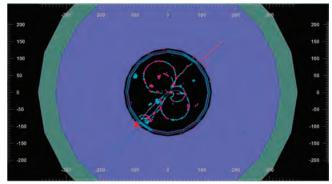


Figure 3: One of the first e+e- collisions recorded by the Belle II detector in March 2018.

the search for processes and particles, not included in the Standard Model (SM), commonly addressed as New Physics (NP); to do so, extremely precise measurement results are confronted to predictions of the SM. While the latter is considered as a very successful effective theory, it is believed that NP must exist and is responsible – among others – for the observed matter–antimatter asymmetry in the universe.

The Belle detector finished taking data in 2010, but analyses of several processes are still ongoing. Among the most noticeable results of the Belle collaboration (537 researchers from 91 institutions and 20 countries) in 2018 are the search for  $B \rightarrow h\nu\nu$  decays (where *h* denotes a light hadron) [3], measurement of semi-tauonic  $B \rightarrow D^*\tau\nu$  decays [4], and the search for  $B \rightarrow \mu\nu$  decays [5].

Semi-leptonic decay  $B \rightarrow h\nu\nu$  is only possible as a higher-order process in the framework of the SM, its branching fraction s predicted to be around 10<sup>-7</sup>. As such it is sensitive to possible NP contributions, specifically to righthanded couplings of neutrinos. The mentioned analysis resulted in so far the most stringent upper limits on the rate of the decay, as presented in Figure 2. The measurement method consists of a reconstruction of one of the *B* mesons from a pair produced in an *e*\**e* collision, enabling reconstruction of the other *B* meson's final state neutrinos. The latter do not interact in the detector and are thus undetectable directly.

A similar method is employed in measurements of  $B \rightarrow D^* \tau v$  decays, which can be used to test the hypothesis of lepton flavor universality, a building block of the SM. The hypothesis predicts identical weak interaction couplings of all the charged leptons ( $\tau$ ,  $\mu$  and e). Measurements of semi-tauonic decays can be compared to decays into lighter leptons ( $\mu$ , e) to test the prediction. While hints of discrepancies exist, the significance of the deviations of theoretical predictions from the experimental results is not yet statistically significant.

The leptonic decay is theoretically well described, although rare (branching fraction approximately  $4 \cdot 10^{-7}$ ). A measurement can be used to determine the  $V_{ub}$  element of the Cabibbo-Kobayashi-Maskawa matrix, and to search for possible contributions of the hypothetical charged Higgs boson. The result of the measurement is a 2.4 standard deviation significant signal with a branching fraction of approximately  $6 \cdot 10^{-7}$ . The significance of the result will be improved in the future by measurements with the Bele II detector.

In 2018 the Belle II detector successfully underwent commissioning and recorded the first data in  $e^*e$  collisions. Analysis of the recorded data in the data-taking period from April to July proves a good operation of the renewed detector, designed to operate at higher luminosity and con-

sequently a harsher background environment. In 2018, also the result of the long-term efforts to build a detailed physics program of the experiment were published [6]. The activities were a joint theory–experiment effort in the framework of Belle II-Theory Interface Platform. An almost 700-page document details the current status and measurement methods for the future Belle II operations and analyses, with the aim f searches for NP.

#### 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<sup>18</sup> eV. In the Earth's atmosphere such particles interact with air nuclei and produce various other parti-

cles. 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 km<sup>2</sup> per century, the Auger Observatory has created a detection area of 3000 km<sup>2</sup> 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 Observatory combines two complementary techniques to measure air showers

The Pierre Auger Collaboration has shown that the energy spectrum of cosmic rays exhibits a sharp drop around 10<sup>20</sup> 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 have already 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 on 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 a Monte Carlo simulation for any reasonable composition mix of cosmic rays.

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 3000-km<sup>2</sup> 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 computing resources of SiGNET Tier-2 in 2018, 6500 CPU cores and 4 PB of storage space, stayed at the same level as in 2017. The usage of CPU resources was 94% and the disk storage at 98%. The computing resources are dedicated to simulation and data deconstruction of data produced with the ATLAS detector and for Monte-Carlo simulation of the Belle II detector; however, a smaller fraction was used by other departments at the Jožef Stefan

Institute and external users in Slovenia. The general purpose NSC cluster at the Jožef Stefan Institute and the computing centre of ARNES are transparently included in distributed computing infrastructure within WLCG collaboration and EGI infrastructure. The arcControlTower system which manages the job execution at ATLAS experiment computing centres was

## The Jožef Stefan Institute is a constitutive member of the Slovenian National Grid Initiative SLING.

further developed in collaboration with the Faculty of Computing and Information Science, and was integrated into the new ATLAS job management system called Harvester. A presentation and publication of the system was given at the CHEP 2018 conference in Sofia, Bulgaria.

The Jožef Stefan Institute is a constitutive member of the Slovenian National Grid Initiative SLING. The SLING consortium was legally established in April 2018 in order to support and leverage the new supercomputing centre HPC-RIVR in Maribor, a nationally funded cohesion-fund project to be fully operational by end of 2020. SiGNET-T2 participated in the design and architecture of HPC-RIVR and will further collaborate in the procurement and development of the system. Slovenia became a member of the EuroHPC project in 2018 to collaborate in the development of a supercomputing infrastructure, where the Jožef Stefan actively participates in the procurement and design of future pre-exascale and peta-scale computing centres. SiGNET-T2 is a full member of international organizations EGI/InSPIRE, wLCG and Nordugrid and has 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

Most of the work on detector development was performed in the framework of the ATLAS and CERN-RD50 collaboration.

We continued the studies of depleted CMOS sensors in 2018, which have been officially accepted by the ATLAS collaboration as the technological option for one layer of pixel detectors of the charged particle tracker after the upgrade of LHC to HL-LHC. Our work concentrated to the measurements of radiation damage effects on the charge collection properties of the CMOS detectors [7] produced by different producers. We established the universal relation between the irradiation fluence and effective doping concentration and made comprehensive studies of the initial dopant removal both with reactor neutron and 24 GeV protons. Most of the studies were done with Edge Transient Current Technique that we pioneered. Furthermore, our measurements clearly showed the necessity of backplane metallization as it affects significantly the charge-collection mechanism. We also took part in several test-beam activities and contributed significantly to the evaluation of these sensors and their assessment of being suitable for the Large Hadron Collider upgrade.

In the past year we continued the work on development of High Granularity Timing Detector for ATLAS. We took the leading role in radiation studies [8] of Low Gain Avalanche Detectors (LGAD), which are the choice for the sensor technology. We have evaluated thin LGADs from several producers and showed that the performance is similar for all. The dependence of gain on fluence was precisely measured in the entire range of HL-LHC fluences and the measured time resolution (50-60 ps per sensor) was also sufficient at the highest fluences, providing <50-mmthick sensors are used. At high fluences the multiplication takes place in silicon bulk as a consequence of the large space charge originating from the irradiation. First measurements of Ga-doped LGADs were performed this year in an attempt to mitigate initial acceptor removal. The radiation tolerance of LGAD is limited to fluences around ~1.5e15 cm<sup>2</sup>, while at higher fluences the operation requires operation very close to the break down voltage. In order to avoid this, an alternative for LGADs was sought in small cell size 3D detectors, which were shown to be radiation hard in the whole HL-LHC range. We showed that these detectors when used with dedicated electronics can reach a time resolution similar to that of the LGADs.

A multichannel system for simultaneous readout of different dosimetric sensors, developed at JSI, was used in the first tests of the dosimetric sensors for online radiation monitoring for ATLAS ITk after the upgrade to HL-LHC.

Our group also took part in an investigation of silicon detectors for the next generation of hadron colliders (e.g., FCC – Future Circular Collider). Work in this field includes measurements of the silicon detector response after exposure to neutron fluences beyond 10<sup>17</sup> ncm<sup>2</sup> and research of methods for dosimetry in extreme radiation environment of future hadron colliders.

In the area of medical detectors, development of PET detector with high spatial resolution was continued within the frame of the CIMA collaboration, a cooperation of researchers from F-9 department with Ohio State University, University of Michigan and IFIC from Valencia. This year images of point sources with different combinations of detectors were recorded.

The accuracy of different detector systems, particularly a collimated gamma camera and a Compton camera in determination of proton range in proton radiotherapy, was determined through simulation. Similar tools were used to evaluate dose distribution in patients in proton radiotherapy with particular stress given to inclusion of involuntary motion during therapy.

Within the framework of the European project AIDA 2020 (Advanced European Infrastructures for Detectors at Accelerators) more than 220 irradiations by neutrons were performed at the reactor centre at the request of 20 different institutions. The focus was on the development of components for planned upgrades of ATLAS, CMS and Belle detectors.

#### Some outstanding publications in the past year

- 1. Aaboud, M. et al., ATLAS Collaboration: *The journal of high energy physics*, 2018, vol. 2018, no. 1, pp. 126-1-126-52
- Aaboud, M. et al., ATLAS Collaboration: *Physics letters. Section B*, ISSN 0370-2693. [Print ed.], 2019, vol. 788, pp. 316-335
- 3. J. Grygier et al. (Belle Coll.), Phys.Rev. D96, 091101 (2017), Addendum: Phys.Rev. D97, 099902 (2018).
- 4. S. Hirose et al. (Belle Coll.), Phys.Rev. D97, 012004 (2018).
- 5. A. Sibidanov et al. (Belle Coll.), Phys.Rev.Lett. 121, 031801 (2018).
- Belle4. E. Kou (ed.) et al., KEK Preprint 2018-27, BELLE2-PUB-PH-2018-001, FERMILAB-PUB-18-398-T, JLAB-THY-18-2780, INT-PUB-18-047, UWThPh 2018-26 (2018).
- I. Mandić et al., "Charge-collection properties of irradiated depleted CMOS pixel test structures", Nucl. Instr. and Meth. A 903 (2018) 126.
- 8. G. Kramberger et al., "Radiation hardness of thin Low Gain Avalanche Detectors", Nucl. Instr. and Meth. A 891 (2018) 68.

#### Awards and Appointments

1. Marko Bračko, Recognition award of the University of Maribor for scientific research project, art and educational work for higher professors, science teachers and other college associates for special successes, achievements and credits, Maribor, Faculty of Chemistry and Chemical Engineering.

#### Organization of Conferences, Congresses and Meetings

- 1. RD42 Workshop, Jožef Stefan Institute, Ljubljana, Slovenia, 12 13 November 2018
- 2. 4th FAST WG3/4/5 Meeting, Jožef Stefan Institute, Ljubljana, Slovenia, 8 9 January 2018

## INTERNATIONAL PROJECTS

- COST TD1401; Fast Advanced Scintillator Timing (FAST) Prof. Peter Križan Cost Office
- COST CA16108 VBSCan; Vector Boson Scattering Coordination and Action Framework Prof. Borut Paul Kerševan Cost Office
- H2020 JENNIFER; Japan and Europe Network for Neutrino and Intensity Frontier Experimental Research
  - Prof. Peter Križan European Commission
- H2020 AIDA-2020; Advanced European Infrastructures for Detectors at Accelerators Prof. Marko Mikuž
- European Commission 5. Development of Solid State Detectors and Readout Electronics for Experimental Particle Physics and Medical Diagnostics
- Physics and Medical Diagnostics Dr. Andrej Gorišek Slovenian Research Agency On Development of Silicon Patterner for Medical Applications
- Development of Silicon Detectors for Medical Applications Prof. Marko Mikuž Slovenian Research Agency
- Fabrication and Qualification of NürFETs Dosimeters for use at Nuclear Reactors Dr. Gregor Kramberger
- Slovenian Research Agency 8. Slovenian Member in Collaboration Board IPPOG - Meeting of Collaboration Board Dr. A. decider Confederation
- Dr. Andrej Gorišek Slovenian Research Agency
- Development of Segmented Silicon and Diamond Radiation Sensors and Readout Electronics for Particle Physics and Medical Diagnostics Asst. Prof. Igor Mandić
  - Slovenian Research Agency
- Study of Portion and Spatial Resolution of High-Resolution Events on Image Quality in Hybrid Resolution PET Systems Prof. Vladimir Cindro
  - Slovenian Research Agency

## RESEARCH PROGRAMS

 Astroparticle Physics Prof. Marko Zavrtanik

## VISITORS FROM ABROAD

- 1. Georgi Gorine, EPFL, Lausanne, Switzerland, 5 3 March 2018
- 2. Giuseppe Pezzullo, Geneva, Switzerland, 5 3 March 2018
- Dr Leonid Burmistrov, Laboratoire de l'Accélérateur, Orsay, France, 5 9 March 2018
   Prof Dr Arie Ruzin, School of Electrical Engineering Faculty of Engineering, Tel Aviv University, Tel Aviv, Israel, 20 - 21 September 2018
- Miloš Manjalović, University of Montenegro, Montenegro, 24 September 5 October 2018
- Dr Rudy Ferraro, CERN European Organization for Nuclear Research, Geneva, Switzerland, 24 - 25 October 2018

2. Experimental Particle Physics Prof. Marko Mikuž

## R & D GRANTS AND CONTRACTS

- History of Doctoral Dissertations by Slovene Candidates in the Austro Hungarian Empire (18721918) Prof. Boštjan Golob
- New atmospheric monitoring devices and techniques for Imaging Atmospheric Cherenkov Telescopes Prof. Marko Zavrtanik
- Depleted CMOS Sensors for the ATLAS Tracker Upgrade and Future Collider Experiments
- Prof. Marko Mikuž 4. Advanced hadron identification methods for Belle II
- Prof. Peter Križan 5. Collaboration CERN RD-39 Prof. Marko Mikuž
- Cern 6. Collaboration CERN RD-50 Prof. Marko Mikuž
- Cern 7. Collaboration DELPHI
- Prof. Borut Paul Kerševan Cern
- 8. Collaboration ATLAS Prof. Marko Mikuž Cern
- Collaboration CERN RD-42 Prof. Marko Mikuž Cern
- Collaborations Belle in Belle II Prof. Peter Križan Kek - High Energy Accelerator Research
- Design, Procurement and QA of Flex-rigid Hybrids Prof. Marko Mikuž
- European Organization for Nuclear Research 12. Irradiations in TRIGA Nuclear Reactor
- Prof. Vladimir Cindro
- Gabriele Piscobo, Laboratoire d'Informatique, de Robotique et de Microélé tronique de Montpellier (LIRMM), Montpellier, France, 24 - 25 October 2018
- Prof Dr Harris Hagan, Ohio State University, Columbus, Ohio, USA, 10 14 November 2018
- 9. Prof Dr William Trischuk, University of Toronto, Ontario, Canada, 10 14 November 2018
- 10. Dr Tomasz Szumlak, AGH Krakow, Krakow, Poland, 12 13 November 2018
- Prof Dr Agnieszka Oblakowska Mucha, AGH Krakow, Krakow, Poland, 12 13 November 2018

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- 19. Asst. Prof. Dejan Žontar\*
- Postdoctoral associates
- 20. Dr. Marko Petrič

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### ORIGINAL ARTICLE

- 1. The Pierre Auger Collaboration, A. Aab *et al.*, "An indication of anisotropy in arrival directions of ultra-high-energy cosmic rays through comparison to the flux pattern of extragalactic gamma-ray sources", *The astrophysical journal. Letters*, 2018, **853**, 2, 1-10.
- The Pierre Auger Collaboration, A. Aab *et al.*, "Large-scale cosmic-ray anisotropies above 4 EeV measured by the Pierre Auger Observatory", *The Astrophysical journal*, 2018, 868, 1, 1-12.
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- 12. ATLAS Collaboration, M. Aaboud *et al.*, "Measurement of differential cross-sections of a single top quark produced in association with a *W*

boson at  $\sqrt{s}$  = 13 TeV with ATLAS", *The European physical journal. C*, 2018, **78**, 3, 186.

21. Dr. Andrej Studen

23. Dania Consuegra Rodriguez, B. Sc.

27. Dr. Miha Muškinja, left 15.10.18

31. Tina Šfiligoj, B. Sc., left 01.10.18

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35. Erik Margan

Note:

Postgraduates

- 13. ATLAS Collaboration, M. Aaboud *et al.*, "Search for doubly charged Higgs boson production in multi-lepton final states with the ATLAS detector using proton-proton collisions at  $\sqrt{s} = 13$  TeV", *The European physical journal. C*, 2018, **78**, 3, 199.
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- 27. ATLAS Collaboration, M. Aaboud *et al.*, "Search for additional heavy neutral Higgs and gauge bosons in the ditau final state produced in  $36 \text{fb}^{-1}$  of *pp* collisions at  $\sqrt{s} = 13$  TeV with the ATLAS detector", *The journal of high energy physics*, 2018, 1, 55.
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- Tomoyuki Konno *et al.* (22 authors), "The aerogel ring image Cherenkov counter for particle identification in the Belle II Experimen", In: Zhen Liu (ed.), *Proceedings of International Conference on Technology and Instrumentation in Particle Physics 2017, 21 - 26 May 2017, Beijing, China. Volume 1*, (Springer proceedings in physics 212) 2018, 270-274.
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### UNIVERSITY, HIGHER EDUCATION OR HIGHER

### VOCATIONAL EDUCATION TEXTBOOK

 Andrej Zorko, Miha Nemevšek, Nejc Košnik, Matic Lubej, Zbirka rešenih nalog iz moderne fizike, Ljubljana: DMFA - založništvo, (Zbirka izbranih poglavij iz fizike 55), 2018.

### MENTORING

- 1. Matic Lubej, *Study of*  $B \rightarrow KKlv_l$  *decays at Belle:* doctoral dissertation, Ljubljana, 2018 (mentor Anže Zupanc).
- 2. Manca Mrvar, Calibration of aerogel ring-imaging Cherenkov detector in Belle II: doctoral dissertation, Ljubljana, 2018 (mentor Rok Pestotnik).
- Miha Muškinja, Search for new physics processes with same charge leptons in the final state with the ATLAS detector: doctoral dissertation, Ljubljana, 2018 (mentor Borut Paul Kerševan; co-mentor Andrej Gorišek).

## 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, the synthesis of new hybrid materials and inorganic materials with special properties. A great deal of the activity of the group has been devoted to technological, ecological and process safety issues 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.



The research of new inorganic compounds containing fluorine was conducted in a study of the reactions between AF (A = Li, Na, K, Rb, Cs) and  $TiF_4$  in anhydrous hydrogen fluoride. Single crystals of five new poly[perfluoridotitanates(IV)] were grown and their crystal structures determined (KTiF<sub>5</sub>, Cs<sub>3</sub>Ti<sub>4</sub>F<sub>19</sub> and [H<sub>3</sub>O]<sub>3</sub>[Ti<sub>6</sub>F<sub>27</sub>], [K,H<sub>3</sub>O]<sub>3</sub>[Ti<sub>6</sub>F<sub>27</sub>], Head:  $[Rb,H_3O]_3[Ti_6F_{27}])$ . The anionic part in the crystal structures of K[TiF\_3] is composed of infinite ( $[TiF_3]^-)\infty$  chains Asst. Prof. Gašper Tavčar built of TiF<sub>6</sub> octahedra sharing joint vertices. The polymeric  $([Ti_6F_{27}]^{3-})_{\infty}$  anion represents the first example of the three-dimensional network built of TiF<sub>6</sub> octahedra. The crystal-structure determination of Cs<sub>2</sub>[Ti<sub>4</sub>F<sub>10</sub>] reveals a new type of polymeric fluoridotitanate(IV) anion, i.e., column-like ( $[Ti_4F_{10}]^{3-}$ ) $\infty$ .

In the research field of the synthesis and characterization of hybrid materials, compounds with fluoridotitanate anions and vanadium oxide fluoride should be highlighted. We studied chemical reactions between guaniStructure of Cs<sub>3</sub>[Ti<sub>4</sub>F<sub>19</sub>] reveals a new type of polymeric fluoridotitanate(IV) anion

dinium carbonate or guanidinium chloride and titanium tetrafluoride. Single-crystal growths from saturated HF, SO, and CH,CN solutions resulted in six new perfluoridotitanate(IV) compounds, which were structurally characterized:  $[C(NH_{2})_{2}]_{2}[TiF_{6}], [C(NH_{2})_{2}]_{4}[Ti_{4}F_{20}], [C(NH_{2})_{2}][Ti_{2}F_{0}], [C(NH_{2})_{2}]_{2}[Ti_{6}F_{27}] \cdot So_{2}, [C(NH_{2})_{2}]_{4}[H_{2}O]_{4}[Ti_{4}F_{20}][TiF_{2}]_{4}$  and  $[H_{5}O_{2}]_{4}[Ti_{8}F_{26}]$ . Their crystal structures consist of monomeric  $[TiF_{6}]^{2-}$ , oligomeric  $[Ti_{4}F_{20}]^{4-}$   $[Ti_{6}F_{27}]^{3-}$  and  $[Ti_{8}F_{26}]^{4-}$ , as well as polymeric ( $[TiF_3]^-$ ) and ( $[TiF_3]^-$ ) perfluoridotitanate(IV) anions. The hexameric  $[TiF_7]^3^-$  anion with a trigonal prismatic geometry was structurally determined for the first time. The crystal-structure determination of the [C(NH<sub>2</sub>),][H<sub>2</sub>O][Ti<sub>4</sub>F<sub>20</sub>][TiF<sub>5</sub>] revealed the first example of a mixed-anion perfluoridotitanate(IV) compound containing two different perfluoridotitanate(IV) anions, i.e., oligomeric  $[Ti_{1}F_{20}]^{4-}$  and 1-D polymeric  $([TiF_{2}]^{-})_{-}$  anions. The crystal structure of the guanidinium hydrogen difluoride salt [C(NH<sub>2</sub>),][HF<sub>2</sub>] was also determined.

Transition-metal oxide fluorides and their anionic analogues are the subject of numerous research papers. Vanadium is one of the transition metals that is in the spotlight of research. It gives a variety of oxide fluoride compounds in different oxidation states (IV, V). With the reaction of vanadium(V) oxide trifluoride (VOF<sub>2</sub>) and the relatively new "naked" fluoride reagent [(L<sup>Dipp</sup>)H][F](L<sup>Dipp</sup> = 1,3-bis(2,6-diisopropylphenyl)-1,3-dihydro-2Himidazol-2-ylidene) we were able to isolate  $[(L^{Dipp})H][VOF_4]$  with the long-sought discrete  $[VOF_{a}]^{-}$  anion. The neutral  $[(L^{Dipp})VOF_{a}]$  complex was synthesized by a similar reaction between VOF, and the bulky N-heterocyclic carbene (NHC) ligand  $L^{Dipp}$ . The hydrolysis of  $[(L^{Dipp})VOF_2]$  led to the  $[(L^{Dipp})$ H][VO,F<sub>2</sub>] salt, which was the most stable product in this system. In cooperation with the Department of Physical and Organic Chemistry we analysed, by means of DFT calculations, intermolecular interactions between [(L<sup>Dipp</sup>) VOF, ] complexes in the crystal structure and realized that these interactions have a significant effect on the V– $F_{trans}$  bond length. We further scrutinized a ligand bonding within the  $[(L^{Dipp})VOF_3]$  and related complexes. We provided the evidence of a minute  $\varpi$  back-bonding into NHC ligands, which is larger for chloride [(NHC)VOCl<sub>2</sub>] than fluoride [(NHC)VOF<sub>2</sub>] complexes, although the fluoride ions are counterintuitively involved in back-bonding. The influence of the  $\varpi$  back-bonding on the V–F  $_{_{trans}}$  and V–F  $_{_{cis}}$  bond lengths was also rationalized.

Figure 1: Discrete  $[VOF_4]^-$  anion in the structure of  $[(L^{Dipp})H][VOF_4]$ ; H atoms are omitted for clarity

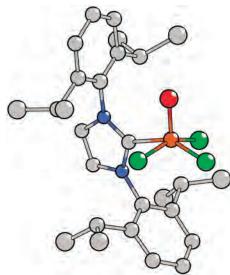


Figure 2: Structure of the neutral  $[(L^{Dipp})]$ VOF<sub>3</sub>] complex; H atoms are omitted for clarity

The reaction of the naked fluoride reagent  $[(L^{Dipp} H][F]$  with VOF<sub>3</sub> leads to the long-sought discrete  $[VOF_4]^-$  anion

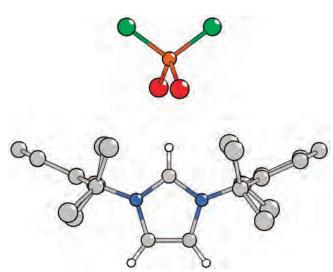


Figure 3: Discrete  $[VO_2F_2]^-$  anion in the structure of  $[(L^{Dipp})H][VO_2F_2]$ ; H atoms are omitted for clarity

In cooperation with a research group from the Ivan Franko National University (Lviv, Ukraine) a number of copper(I) pi-complexes with heterocyclic ligands were obtained and explored. The structural characterization of the first-known copper(I) azide pi-complex should be highlighted. Bi-metallic copper-calcium and copper-barium complexes with *in-situ*-formed ligands were obtained and investigated in collaboration with the Taras Shevchenko Kyiv National University (Kyiv, Ukraine). Re-crystallisation of the mixture of copper(II) chloride and *dabco* (*dabco* = 1,4-diazabicyclo [2.2.2] octane) resulted in the formation of (H,*dabco*)<sub>5</sub>(CuCl<sub>4</sub>)<sub>4</sub>CuCl<sub>4</sub>(H,O)<sub>2</sub> and (H,*dabco*)Cu<sub>2</sub>Cl<sub>6</sub> salts.

We should also mention activities from the analytical, technological, ecological and process-safety-issues research areas of the department. We analysed samples and the products of gasification of diverse solid waste materials and the impact of diverse alkaline additives on the gasification and concentration of the unwanted substances of the synthesis gas. In addition, we studied the optimal process conditions for the transformation of a model tar substance (toluene) via catalytic oxidation and steam reforming to a synthesis gas, as well as the preparation of the related catalyst.

The thermochemistry of reactions proceeding during the most frequently used decomposition methods (i.e., pyrohydrolysis, oxygen bomb combustion and alkaline carbonate fusion) for a subsequent determination of fluorine by fluoride ion selective electrode was investigated. Within the topic of process safety, in 2018 we researched and published work on the topics

of the evaluation of the quality of the management of changes in industrial organizations, as well as on the relations among the safety-management systems and the leadership styles in the mentioned organizations. We continued and successfully completed the technical lead of one of the phases of the consultation project for an industrial client outside Slovenia (it was about the implementation of the element of the safety management of technical and organizational changes in a rather large organization in the oil and gas industry).

We continued with our activity in the field of education and the promotion of sciences. 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 schools, secondary schools and even kindergartens through experimental courses performed in a specialized laboratory or through direct demonstrations at the schools. With demonstrations of chemical experiments, we participated at the Hokus pokus, Lupa festival, Slovenian Science Festival, organized by the Slovenian Science Foundation and at the Researchers' Night. Some of the activities of the School of Experimental Chemistry were carried out within the project, which is funded by the JSI and the City of Ljubljana.

### Some outstanding publications in the past year

- 1. I. Shlyapnikov, E. A. Goreshnik, Z. Mazej, Increasing structural dimensionality of alkali metal fluoridotitanates(IV), *Inorganic chemistry*, 57 (2018) 1976-1987.
- Ž. Zupanek, M. Tramšek, A. Kokalj, G. Tavčar, Reactivity of VOF<sub>3</sub> with N-heterocyclic carbene and imidazolium fluoride: analysis of ligand–VOF<sub>3</sub> bonding with evidence of a minute *σ* back-donation of fluoride, *Inorganic chemistry*, 57 (2018) 13866-13879.
- Shlyapnikov, E. A. Goreshnik, Z. Mazej, Guanidinium perfluoridotitanate(IV) compounds : structural determination of an oligomeric [Ti<sub>6</sub>F<sub>27</sub>]<sup>3–</sup> anion, and an example of a mixed-anion salt containing two different fluoridotitanate(IV) anions, *European Journal of Inorganic Chemistry*, (2018) 5246-5257.
- D. Štepec, M. Ponikvar-Svet, J. F. Liebman, Paradoxes and paradigms: observations on pyrohydrolysis, oxygen bomb combustion, and alkaline carbonate fusion, most frequently used decomposition methods for subsequent determination of fluorine and accompanying thermochemistry, *Structural chemistry*, 29 (2018) 1247-1254.
- 5. D. Levovnik, M. Gerbec, Operational readiness for the integrated management of changes in the industrial organizations: assessment approach and results, *Safety science*, 107 (2018) 119-129.

#### Annual Report 2018

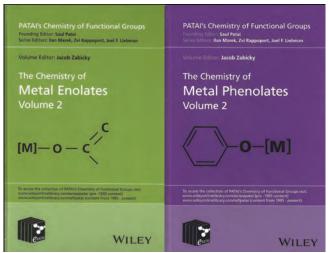


Figure 4: Maja Ponikvar-Svet, with co-authors, contributed chapters to the books "The Chemistry of Metal Enolates" (a) and "The Chemistry of the Metal Phenolates" (b) published by Wiley in 2018

### INTERNATIONAL PROJECTS

- 1. Extraction of Tantalum and Niobium from Ores Asst. Prof. Gašper Tavčar Prg Ltd.
- Implementation of Process Safety Management System (PSMS) into NIS j.s.c. 2. Prof. Marko Gerbec
- European Virtual Institute For Integrated Risk
- H2020 NOCMOC; European Researchers' Night (NIGHT) 3. Dr. Melita Tramšek European Commission
- The Development of a Nondestructive Analytical Method for the Screening of 4. Upconverting Nanoparticles Surface Properties Based on Optical Characterization Prof. Maja Ponikvar-svet Slovenian Research Agency

### **RESEARCH PROGRAM**

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

### **STAFF**

- Researchers
- Prof. Marko Gerbec 1.
- Asst. Prof. Evgeny Goreshnik Dr. Adolf Jesih, retired 29.03.18
- 3. Dr. Robert Kocjančič 4.
- Dr. Zoran Mazej 5.
- Prof. Maja Ponikvar-Svet 6.
- Asst. Prof. Tomaž Skapin 7.
- Asst. Prof. Gašper Tavčar, Head 8
- 9. Dr. Melita Tramšek
- Postdoctoral associate
- 10 Dr Blaž Alič
- Postgraduates
- 11. Evelin Gruden, B. Sc.

### VISITOR FROM ABROAD

1. Mateusz Winny, Student exchange, University of Warsaw, Warsaw, Poland, 27. 8.-14. 9. 2018



Figure 5: The School of Experimental Chemistry presented interesting experiments at the Researchers' Night event (photograph. B. Alič)

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

- Direct Conversion of Methane to Higher Hydrocarbons Using Superacid Catalysts 1 Asst. Prof. Gašper Tavčar
- 2 Evaluation of greenhouse gasses mitigation measures in industry Dr. Robert Kocjančič
- SUstainability PERformance of LNG-basedmaritime mobility 3. Prof. Marko Gerbec Rhe Emillia-romagna Region
- Evaluation of greenhouse gasses mitigation measures in industry 4 Dr. Robert Kocjančič Ministry of the Environment and Spatial Planning

### NEW CONTRACT

- 1. Research and development of the gasification technology services Prof. Marko Gerbec Syntech d. o. o.
- 12. David Levovnik, B. Sc. 13. Yaryna Soyka, B. Sc. 14. Dona Štepec, B. Sc. 15. Žiga Zupanek, B. Sc. Technical officers 16. Tine Oblak, M. Sc. 17. Tomaž Ogrin, M. Sc. Technical and administrative staff 18. Peter Frkal. B. Sc. 19. Pero Kolobarić 20. Robert Moravec
- 21. Mira Zupančič

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### **ORIGINAL ARTICLE**

- 1. Bojana Višić, Eva Kranjc, Luka Pirker, Urška Bačnik, Gašper Tavčar, Srečo D. Škapin, Maja Remškar, "Incense powder and particle emission characteristics during and after burning incense in an unventilated room setting", *Air quality, atmosphere & health*, 2018, **11**, 6, 649-663.
- Majda Pavlin, Radojko Jaćimović, Andrej Stergaršek, Peter Frkal, Maja Koblar, Milena Horvat, "Distribution and accumulation of major and trace elements in gypsum samples from lignite combustion power plant", *American journal of analytical chemistry*, 2018, 9, 602-621.
- 3. Yurii Slyvka, A. A. Fedorchuk, Evgeny A. Goreshnik, G. Lakshminarayana, I. V. Kityk, P. Czaja, Marian G. Mys'kiv, "Synthesis, structural and NLO properties of the novel copper(I) p-toluenesulfonate  $\pi$ -complex with 1-allyloxybenzotriazole", *Chemical Physics Letters*, 2018, **694**, 112-119.
- Urška Vrabič Brodnjak, Adolf Jesih, Diana Gregor-Svetec, "Chitosan based regenerated cellulose fibers functionalized with plasma and ultrasound", *Coatings*, April 2018, 8, 4, 133.
- Samuel Rodman Oprešnik, Rok Vihar, Tine Seljak, Rok Vihar, Marko Gerbec, Tomaž Katrašnik, "Real-World fuel consumption, fuel cost and exhaust emissions of different bus powertrain technologies", *Energies*, 2018, **11**, 8, 2160.
- 6. Igor Shlyapnikov, Evgeny A. Goreshnik, Zoran Mazej, "Guanidinium perfluoridotitanate(IV) compounds: structural determination of an oligomeric  $[Ti_6F_{27}]^{3-}$  anion, and an example of a mixed-anion salt containing two different fluoridotitanate(IV) anions", *European Journal of Inorganic Chemistry*, 2018, 48, 5246-5257.
- 7. Igor Shlyapnikov, Evgeny A. Goreshnik, Zoran Mazej, "Increasing structural dimensionality of alkali metal fluoridotitanates(IV)", *Inorganic chemistry*, 2018, **57**, 4, 1976-1987.
- 8. Žiga Zupanek, Melita Tramšek, Anton Kokalj, Gašper Tavčar, "Reactivity of VOF<sub>3</sub> with N-heterocyclic carbene and imidazolium fluoride: analysis of ligand-VOF<sub>3</sub> bonding with evidence of a minute-back-donation of fluoride", *Inorganic chemistry*, 2018, **57**, 21, 13866-13879.
- 9. Andrii Vakulka, Evgeny A. Goreshnik, "Copper(I) bromide and chloride complexes with urotropine and triethylenediamine: synthesis, crystal structure, and Raman characterization", *Journal of coordination chemistry*, 2018, **71**, 15, 1426-2440.
- 10. A. A. Fedorchuk, Yurii Slyvka, Evgeny A. Goreshnik, I. V. Kityk, P. Czaja, Marian G. Mys'kiv, "Crystal structure and NLO properties of the novel

tetranuclear copper(I) chloride  $\pi$ -complex with 3-allyl-2-(allylimino)-1,3-thiazolidin-4-one", *Journal of molecular structure*, 2018, **1171**, 644-649.

- 11. Biljana Kiteska, Nenad Funduk, Pavel Cevc, Adolf Jesih, Alojz Anžlovar, Igor Kopač, "The influence of free-radical concentration on the shear bond strength of dental composites", *Materiali in tehnologije*, 2018, **52**, 2, 177-182.
- 12. Matej Prijatelj, Nataša Čelan Korošin, Tomaž Skapin, Victor Vega Mayoral, Daniele Vella, Janez Kovač, Dragan Mihailović, Christoph Gadermaier, "Preparation of air-stable expandable MoS<sub>2</sub> and rapid expansion by low temperature heating and electron beam irradiation", *Materials letters*, 2018, **218**, 229-232.
- 13. Ljupka Stojchevska, Petra Šutar, Evgeny A. Goreshnik, Dragan Mihailović, Tomaž Mertelj, "Stability of the light-induced hidden charge density wave state within the phase diagram of  $1T TaS_{2-x}Se_x$ ", *Physical review. B*, 2018, **98**, 19, 195121.
- 14. David Levovnik, Marko Gerbec, "Operational readiness for the integrated management of changes in the industrial organizations: assessment approach and results", *Safety science*, 2018, **107**, 119-129.
- 15. Dona Štepec, Maja Ponikvar-Svet, Joel F. Liebman, "Paradoxes and paradigms: observations on pyrohydrolysis, oxygen bomb combustion, and alkaline carbonate fusion, most frequently used decomposition methods for subsequent determination of fluorine and accompanying thermochemistry", *Structural chemistry*, 2018, **29**, 5, 1247-1254.
- 16. Olga Shyyka, Nazariy Pokhodylo, Yurii Slyvka, Evgeny A. Goreshnik, Mykola Obushak, "Understanding the tetrazole ring cleavage reaction with hydrazines: structural determination and mechanistic insight", *Tetrahedron letters*, 2018, **59**, 12, 1112-1115.

### **REVIEW ARTICLE**

- 1. Maja Ponikvar-Svet, Diana N. Zeiger, Joel F. Liebman, "Interplay of thermochemistry and Structural Chemistry, the journal (volume 28, 2017, issues 1-2) and the discipline", *Structural chemistry*, 2018, **29**, 3, 947-955.
- 2. Maja Ponikvar-Svet, Diana N. Zeiger, Joel F. Liebman, "Interplay of thermochemistry and Structural Chemistry, the journal (volume 28, 2018, issues 3-4) and the discipline", *Structural chemistry*, 2018, **29**, 4, 1235-1245.

## DEPARTMENT OF PHYSICAL AND ORGANIC CHEMISTRY K-3

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

Our experimental and theoretical investigations of elementary physico-chemical processes on solid surfaces are mainly focused in the field of corrosion, corrosion protection and catalysis. Corrosion is a widespread phenomenon with significant economic and environmental impacts. Because of the enormous costs, the protection of metals and alloys is therefore essential. In-depth basic knowledge of surface processes is needed to design effective corrosion protection since the understanding of the mechanism of inhibition of corrosion at the atomic level is still very limited. In order to overcome this, we introduced a synergistic iterative research, combining the synthesis of new compounds, electrochemical and surface analytical techniques, and the modelling and simulation of processes based on the first principles. Such a newly established research strategy is expected to boost the innovative design of advanced sustainable solutions in the protection of materials.



Prof. Ingrid Milošev

We are mainly focused on alloys based on aluminium and copper, as well as steel and other technologically important materials. Lightweight aluminium alloys are used in various applications, especially in the transport industry, where there is a great need to reduce the weight of vehicles and consequently reduce emissions into the environment. Steel and alloys based on copper are indispensable materials in the field of infrastructure, construction,

etc. Traditional ways of corrosion protection such as conversion chromate coatings can no longer be used due to ecological restrictions. Over the past decade, various alternatives have been explored, among which the most important are sol-gel coatings, conversion coatings, superhydrophobic coatings and various inorganic and organic inhibitors. The needs of industry, in particular transport, construction, machine and electronics, postulate the requirements for development of efficient, sustainable and environmentally friendly coatings, which at the same time exhibit additional functional characteristics. In our laboratory, we investigate all of the above-mentioned alternatives and even combine them with each other, e.g. sol-gel coatings and inhibitors in order to achieve not only barrier protection, but also active protection, where the coating after corrosion damage is able to self-heal. We also introduce modern methodologies, such as the atomic layer deposition, in corrosion protection.

Conversion coatings based on the salts of rare earths, zirconium or titanium are an important research direction in the search for novel corrosion protection. A prominent article on zirconium and / or titanium conversion coatings was published in the reputable Journal of the Electrochemical Society prepared by I. Milošev and G.S. Frankel (Fontana Corrosion Center, The Ohio State University, USA). Conversion coatings based on Zr and/or Ti are alternative to chromate and phosphate coating technologies that can be associated with environmental problems. In the review article, scientific achievements in this rapidly evolving field are covered, offering a description of the composition of the conversion baths, mechanisms of the coating deposition and coating characterization. The protective properties of these coatings are also reviewed. In 2018, this review article was the most downloaded article in the Journal of The Electrochemical Society, section "Corrosion Science and Technology". We continue our own research in the field of conversion coatings prepared from the zirconium hexafluoride bath. The coating formation process involves activating the surface in an acidic fluoride-containing medium. This step is followed by precipitation of Zr-based oxide at cathodic regions on the surface where the

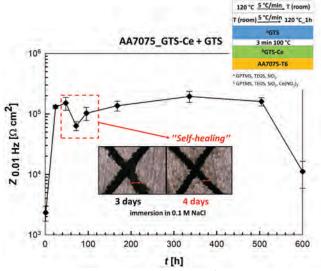


Figure 1: Impedance at 0.01 Hz determined from the electrochemical impedance spectra recorded in 0.1 M NaCl solution during the immersion of the hybrid sol-gel GTS-Ce coating on aluminium alloy AA7075-T6. The course of impedance during the course of immersion indicates that the coating self-heals. Namely, after an initial drop, after four days, the impedance increased and remains unchanged for 500 hours. The diameter of artificial corrosion damage decreased after four days. Structure of the coating and curing scheme are shown in the inset.

Cerium ions added to hybrid sol-gel coatings increase the coating density and bring the selfhealing ability after corrosion damage resulting in exceptional anti-corrosion protection of aluminium alloys in a corrosive medium. pH increases due to the reduction of oxygen. The increase in pH causes the deposition of metal oxide, i.e., conversion of the hexafluoro zirconic acid to the zirconium hydrated oxide. The effect of the parameters of the conversion bath on the efficiency of the corrosion protection of zirconium conversion coatings deposited on different aluminium alloys, from the series 3xxx, 4xxx, 5xxx, 6xxx and 7xxx, are investigated. The purpose of the study is to determine the influence of the substrate, especially the type of intermetallic particles, on the properties of conversion coatings. On the basis of this study, we expect to postulate in more detail the mechanism of conversion and formation of a coating. Further, we explore various commercially available conversion coatings based on trivalent chromium or

CorrTalk Workshop was held in June 2018 at the Jožef Stefan Institute organized by doc. dr. A. Kokalj, prof. dr. I. Milošev and mag. D. Lorber. The workshop was devoted to integrative approaches in the investigation of corrosion and inhibition of corrosion. The workshop was held under the auspices of M-Era.Net and was attended by eminent European experts from the field of corrosion, surface analysis and modelling as invited lecturers. zirconium, which are available on the market as an alternative to chromate coatings. As a substrate, aluminium alloy from the series 3xxx important in the construction industry is used. The deposition procedure of various commercial coatings is being optimized depending on the pre-treatment of the surface of the aluminium alloy and then characterized in terms of corrosion protection, microstructure and composition.

A very important part of our research comprises various hybrid solgel coatings designed to protect aluminium alloys or steel in a chloride environment. We are currently investigating four types of coatings in our laboratory, which are designated as GTS and GTS-Ce, TMZ, TMM and ZG. For the preparation of hybrid, i.e., inorganic-organic, silicon sol-gel GTS coatings, precursors tetraethyl orthosilicate (TEOS) and organically

modified silane precursor 3-glycidoxypropyl trimethoxysilane (GPTMS) are used. The sol also contains particles of silicon dioxide to achieve the barrier properties of the coating. To achieve the inhibition properties, cerium(III) nitrate is added to sol (GTS-Ce label). The optimization of the sol synthesis was based on the results of ATR-FTIR

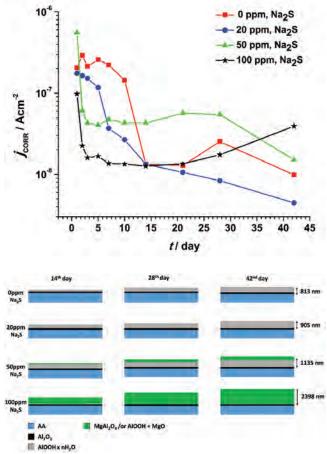


Figure 2: The density of the corrosion current in dependence on the immersion time measured on the samples of AlSi7Mg0.3 alloy in artificial sea water with and without Na s added in the concentration range between 0 and 100 ppm (top panel). A schematic representation of the formation of an oxide layer formed on the surface of the alloy AlSi7Mg0.3 in seawater as a function of the immersion time (lower panel).

properties of the coating. To achieve the initiation properties, certain(iii) he optimization of the sol synthesis was based on the results of ATR-FTIR and UV-vis-NIR spectroscopy. We confirmed the opening of epoxy rings and the completion of hydrolysis and the condensation reaction during the synthesis process. During the synthesis of the sol, a high degree of crosslinking of the Si–O–Si structure and, consequently, a high density of the coating was achieved. Coatings were deposited on aluminium alloy AA7075-T6 using a dip coater. Thickness, contact angle of water drops, roughness and adhesion of coatings to the substrate were determined. The condensation process and the incorporation of cerium nitrate into the hybrid sol-gel coating affect the corrosion properties of the coating. The observed increase in the degree of corrosion protection is attributed to the combination of the barrier properties of silicon matrix with the active protection of cerium nitrate.

A multilayer coating consisting of the first layer of GTS-Ce doped with  $Ce(NO_3)_3$  and other, non-doped GTS layer was also prepared. The addition of cerium ions increases the lifetime of the hybrid coating and plays a role in the self-healing only if it is locked in the first layer of a multi-layer coating. Self-healing is described as the possibility of self-regeneration of the coating after corrosion damage. On the surface of the coated substrates we intentionally made artificial corrosion damage and then monitored the course of self-healing of the coating in a 0.1-M NaCl solution. This process is based on the transport of cerium(III) ions to the site of damage and their oxidation and deposition as insoluble Ce(IV) oxide. The course of self-healing was monitored by electrochemical impedance spectroscopy, X-ray photoelectron spectroscopy and scanning electron microscopy with chemical analysis.

The other type of hybrid sol-gel coatings developed in the laboratory are TMZ coatings prepared from TEOS and an organically modified silane precursor of 3-methacryloxy propyltrimethoxysilane (MAPTMS), which was then mixed with different amounts of zirconium(IV) propoxide, chelated with methacrylic acid. Synthesized coatings are composed of silicon and zirconium oxides in polymerized organic matrix. Due to their density and low porosity, they offer a high level of barrier protection. In these coatings, we also investigated the possibility of self-healing. The focus was on the synthesis and characterization of TMZ coatings with and without the addition of cerium(III) ions. The coatings were applied to aluminium. The chemical composition, structure, thermal properties and porosity of non-doped and Ce-doped coatings containing various concentrations of Zr were analysed by Raman spectroscopy and photothermal beam deflection spectroscopy. The corrosion properties of Al with the TMZ coating were assessed using AC and DC electrochemical methods in a 0.1 M NaCl solution. Barrier and protective properties of the coatings were followed during long-term immersion into the chloride solution using electrochemical impedance spectroscopy. The effect of cerium ions was twofold: cerium influences the formation of a more condensed structure Si–O–Zr, Si–O–Si and Si–O–Al, as well as the formation of Ce-oxide deposits at the interface coating/substrate. The latter leads to the degree of cathodic reaction and hence the degree of corrosion. The synergistic effect of cerium created the coating that acts as an effective barrier and shows active corrosion protection.

In addition, we studied the study of the mechanism of synthesis of TMZ coatings using in-situ FTIR spectroscopy and <sup>1</sup>H, <sup>13</sup>C and <sup>29</sup>Si NMR spectroscopy in dependence on the Zr content of the coating. The following properties of the coating were analysed: transparency, topography, chemical composition, morphology and wettability. The corrosion properties were assessed using electrochemical methods in 0.1-M NaCl solution in a pH range of 3 to 10. The chemical stability of the coatings was also evaluated in a strong alkaline solution. The prepared coatings are transparent and increase the wettability of the water drop for both polar and nonpolar liquids. Electrochemical measurements confirmed the exceptional protection of TMZ coatings in NaCl solutions of various pH, especially those with a high Zr /Si ratio.

We also continue to work on the development of sol-gel polysiloxane TMM coatings based on TEOS, MAPTMS and methacrylates with different lengths of the alkyl chain. The aim is to produce coatings which, in addition to anti-corrosion properties, will also show increased hydrophobicity, which is important in the applications of metal materials in the sea. Namely, once immersed in sea, every artificial surface is subjected to fouling and the formation of a biofilm. It begins with adsorption of bacteria and increases to the formation of algae, micro- and macro-organisms. Therefore, anti-fouling protection is a growing area for application of new materials. Field testing of new coatings for their antifouling ability is carried out in cooperation with the Marine Biology Station of the National Institute of Biology in Piran. Sol-gel coatings, which were developed in our laboratory, were applied to various aluminium alloys and tested in the Adriatic Sea for 8 months. Field test was preceded by an extensive study of the corrosion mechanism of aluminium alloy in laboratory conditions in the artificial sea. Aluminium alloy AlSi7Mg0.3 is intended for applications in seawater, especially parts of motor boats. In particular, we investigated the influence of the presence of sulphide ions in artificial sea water. Sulphides are one of the most common pollutants in natural seawater and can reach levels of 50 ppm or more in heavily contaminated coastal or port waters. In unpolluted natural seawater, a sulphide concentration of 2-7 ppm was reported. Laboratory immersion test lasted 42 days and was performed in artificial sea water with Na<sub>2</sub>S added in concentration between 0 and 100 ppm. Samples were taken at different times and then analysed in terms of electrochemical and microstructural properties. The density of the corrosion current for samples immersed in all solutions tested was very low, ranging from 10-7 to 10-9 A cm-2. The structure, composition and degree of protection of the resulting oxide layers were dependent on the

By means of an integrative approach consisting of electrochemical testing, surface science experiments, and computational DFT modelling, we showed that linear carboxylic acids have the ability to make aluminium superhydrophobic and to enhance its corrosion resistance, provided that their alkyl chains are long enough, because they make the protective organic film stable.

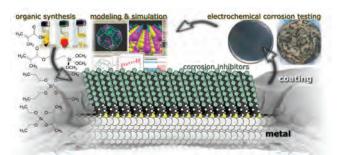


Figure 3: The needs of industry growingly postulate the requirements for development of efficient, sustainable and environmentally friendly corrosion protection. Schematic presentation of a synergistic iterative approach where organic synthesis, electrochemical and surface-science techniques as well as atomistic first-principle-based modelling and simulation are utilized. The modelling and experiments are therefore combined by an integrative approach to boost research and development of new protection means.



Figure 4: Cartoon of impermeability of the organic film composed of linear carboxylic acids on aluminium substrate, illustrating how the effective molecular coverage increases with the length of the alkyl chain. Top row: molecules with shorter alkyl chains do not completely cover the surface (notice uncovered patches of the surface). However, for molecules with longer alkyl chains the surface is effectively covered due to molecular tilting. This effect is schematically depicted by side-view sketches in the bottom row.

concentration of Na<sub>2</sub>S and the time of immersion. We found that, unlike some other materials, for example steels, the presence of a low sulphide concentration (<50 ppm) is useful for corrosion protection of the alloy AlSi7Mg0.3.

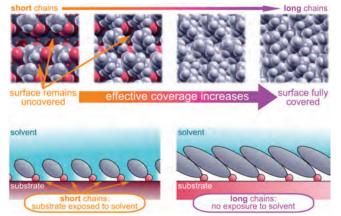


Figure 5: In June 2018 an international workshop CorrTalk was organized at the Department of Physical and organic chemistry of the Jožef Stefan Institute. Workshop was devoted to integrative approaches in the investigation of corrosion and inhibition of corrosion. It was held under the auspices of M.Era.Net and was attended by top European experts from the field of corrosion, surface analysis and modelling as invited lecturers.

The superior activity of silver nanoparticles in the formation of methyl-formate from CO<sub>2</sub>, H<sub>2</sub>, and CH<sub>3</sub>OH stems from their ability to bind atomic hydrogen weakly and surface formate intermediates strong enough.

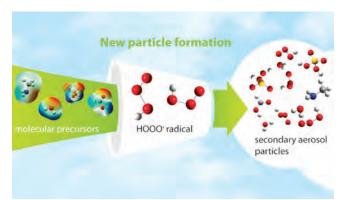


Figure 6: Schematic representation of new aerosol particle formation in the troposphere from molecular precursors and H000 • radical.

This was attributed to the formation of a multilayer oxide layer which, in addition to aluminium hydrated oxide, also contains magnesium oxide.

We continued to work on the 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 aluminum alloys with targeted properties of increased corrosion resistance, specific hydrophobic properties, prolonged service life-time and reduced ecological impact. 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, Chimie ParisTech (CNRS) from Paris and Eötvös Loránd University from Budapest. 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. The current state-of-the-art in this field is represented by high throughput experimental empirical testing of large sets of organic compounds. In contrast to such trial and error approach, a rational design of new corrosion inhibitors would provide a major breakthrough in the field of corrosion protection. The scientific framework should therefore postulate the strategy which will contribute to the increased understanding of corrosion inhibition. One of the possibility is to use the ICME (Integrated Computational Materials Engineering) principles. The basic relationships between aluminium surface and corrosion inhibitors are therefore addressed, i.e. corrosion inhibitors were designed in such a way to allow the investigation of the effect of anchor group and the effect of backbone chain on their inhibitive performance on aluminium in chloride solution. Methodological approach was versatile: (i) synthesis or purchase of organic inhibitors, (ii) preparation of uncoated and inhibitor-coated aluminium samples, (iii) electrochemical measurements, (iv) water contact angle measurements (v) long-term immersion tests, (vi) surface analytical study by SEM, ToF-SIMS or XPS, and (vii) Density Functional Theory (DFT) modeling. The surface of aluminium substrates was prepared by alkaline etching to allow easy self-assembling during immersion in ethanol solution of selected corrosion inhibitors. The inhibitors differed in the (i) type of backbone chain, (ii) length of backbone chain, and (iii) type of anchor group. Based on the obtained experimental (electrochemical parameters and composition of the surface layers) and computational (adsorption reaction energies decomposed into inhibitor-surface and lateral inhibitorinhibitor interactions, adsorption induced changes of electronic structure, etc.) parameters we are aiming to build a predictive model for screening new corrosion inhibitors with targeted properties. The modelling and experiments are therefore combined by an integrative approach.

DFT calculations were also employed to supplement the systematic experimental study on the effect of the length of the alkyl chains on the corrosion inhibition performance of carboxylic acids (CAs) on aluminium in chloride solution. Strong adhesion of the organic film to the surface is often assumed to be a key factor in achieving good corrosion inhibition and to this end, the adsorption of CAs, with alkyl chain lengths from 2 to 18 carbon atoms, was considered on a model of the fully hydroxylated aluminium surface. We found that adsorption of short-chain carboxylic acids is only marginally exothermic, indicating that an additional stabilization is required for them to form a stable adsorbed monolayer. Such a stabilization can be achieved by increasing the length of the alkyl chain, because longer chains provide stronger cohesion via lateral inter-molecular dispersive interactions. Lateral cohesive inter-molecular interactions are further enhanced by the alkyl chain tilting. Apart from increasing cohesion, such tilting also increases the effective coverage of the surface thus preventing the solvent molecules and aggressive species from reaching the substrate.

Within the project COR\_ID we also develop siloxane coatings for use on aluminium alloys, which are exposed to aggressive conditions, such as seawater or dirty water. Under these conditions it is important that the surface is hydro- or superhydrophobic. This may be achieved by the addition of fluorine compounds to the siloxane coating.

Laboratory testing of coatings is being upgraded in collaboration with the company Talum d.d by constructing the pilot device for industrial conditions.

In the context of providing atomistic level insight into the mechanism by which siloxane based sol-gel coatings adhere to Al substrates we studied the adsorption of a model silanol molecule, CH<sub>3</sub>Si(OH)<sub>3</sub>, and its oligomers (up to the trimer) on oxidized and fully-hydroxylated aluminium substrates by means of DFT modelling. We found that

the reaction with the hydroxylated surface via the condensation mechanism—where the silanol molecule replaces a surface OH group, forming a water molecule as a co-product and a strong SiO—Al chemical bond with the surface (monodentate bonding mode)—is both exothermic and exergonic irrespective of oligomer size. However, the formation of a second such bond (bidentate bonding mode) was found thermodynamically unfavourable for the monomer, athermic for the dimer, and favourable for the trimer.

Quantum-chemical calculations indicate that secondary aerosol complexes can be identified by IR spectroscopy, which can aid in faster atmospheric particles identification.

Our calculations therefore indicate that a silanol unit can form at most one strong SiO–Al bond with the surface in the siloxane film. Moreover, some silanol units likely act as spacers as to reduce the overall strain induced by adsorption on the aluminium based substrate.

We continued to work on the M-Era.Net project entitled "COIN DESC: Corrosion inhibition and dealloying descriptors". The specific objective of the project is to identify physically-sound corrosion inhibition and dealloying descriptors, depending on the metallic material and environment to which the material is exposed. Such descriptors are mandatory for the construction of a new corrosion inhibitor virtual design framework which will allow a faster and more rational screening of new specifically designed corrosion inhibitors with superior

characteristics. The project consortium consists of four partners from Slovenia, Belgium, Spain, and Netherlands (Department of Physical and Organic Chemistry of Jožef Stefan Institute, Institute for Materials Research of Hasselt University, Department of Physics at Universitat Politècnica de Catalunya, and Materials Science and Engineering at Delft University of Technology). To this end, we have tested about two dozen of different azole molecules as potential corrosion inhibitors for copper and zinc in NaCl solution by electrochemical methods, such as polarization resistance and electrochemical impedance spectroscopy. The interfacial bonding of inhibitors was investigated by FTIR, XPS, and AFM techniques as well as by explicit DFT inhibitor-surface calculations. We aim at integrating highthroughput oriented experimental testing of a larger number of corrosion inhibitors with insights provided from more detailed mechanistic analyses (experimental and computational) with the specific objective to identify

(experimental and computational) with the specific objective to identify physically-sound corrosion inhibition descriptors. Further scrutiny was devoted to a detailed characterization of adsorption bonding of imidazole, triazole, and tetrazole inhibitors to oxidized copper surfaces. We showed that dissociative adsorption bonding of imidazoles differs considerably from that of triazoles and tetrazoles. While for the latter two dissociative adsorption proceeds via the cleavage of the N–H bond without any significant activation barrier, such a mode is thermodynamically unfavourable for imidazoles. Instead, imidazoles may adsorb dissociatively via the cleavage of the C–H bond. However, such a dissociation is kinetically hindered, because the respective activation barrier is about 1.1 eV.

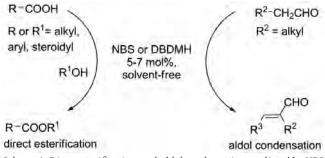
In the field of heterogeneous catalysis, we explained with aid of DFT modelling why silver nanoparticles, supported on sillica-support, were found significantly more active for the continuous methyl-formate synthesis than

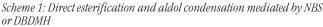
the known gold and copper catalysts. In particular, a careful analysis of results of DFT simulations allowed us to attribute the high activity of silver in synthesis of methyl-formate from  $CO_2$ ,  $H_2$ , and  $CH_3OH$  to its superior ability to form surface formates and formic acid intermediates. We found that the respective activation barrier is given by the interplay between weak

Direct esterification of carbocyclic acids and aldol condensation could be achieved by NBS or DBDMH catalysed reactions under solvent-free conditions.

and strong adsorption bonding of atomic hydrogen and formate, respectively. Among the coinage metals, silver displays the lowest activation barrier for the formation of formates, because it binds atomic hydrogen weakly and formates strong enough, whereas gold binds formates too weakly and copper binds H too strongly.

We also continued with our research in the field of atmospheric chemistry and studied secondary aerosol clusters, which are known to represent nucleation centres for the growth of new particles produced by the agglomeration of various gaseous molecules in the atmosphere. We investigated by quantum-chemical modelling the stability and reactivity of the hydrotrioxy radical (HOOO<sup>•</sup>), because its existence in the atmosphere is controversial and only a few studies have examined its impact on the new aerosol particle formation. In particular, we addressed the formation of binary and ternary complexes of hydrotrioxy radical under troposphere conditions with known atmospheric





precursors, such as aqueous vapour, methanoic acid, methylamine and sulfuric(VI) acid. We found that complexes of HOOO<sup>•</sup> radical and sulfuric(VI) acid are formed spontaneously. On the basis of calculated anharmonic frequencies of the relevant complexes, we have shown that they can be identified by IR spectroscopy, which can aid in faster atmospheric particles identification.

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. Our recent discovery, that organic compounds bearing an active N-halo bond are potential catalysts for several transformations of organic molecules, was used as an original approach for the aldol condensation of comprehensive type of alkyl aldehydes. The reactions could be performed under solvent-free reaction conditions using substoichiometric amounts (5-7 mol %) of N-bromosuccinimide (NBS) or 1,3-dibromo-5,5-dimethyl hidantoine (DBDMH) as the catalysts. In the case of reactions of single aldehyde bearing metylenic functionality near the aldehyde functional group, the self-condensation took place, resulting in the formation of corresponding E-1,2-dialkyl unsaturated aldehyde derivatives. We succeeded in considerable selective cross-condensation of benzaldehydes and alkyl aldehydes and by optimal reaction conditions reduced the self-condensation side reaction to not more than 10%.

The new method of NBS mediated direct esterification of carbocyclic acids was improved by the use of lower cost DBDMH as the catalyst thus achieving selective and efficient esterification of benzoic, mono-, di-, and tri-alkyl carboxylic acids and few steroid analogues bearing carboxy or hydroxy functionalization.

In collaboration with University of North Florida and Universidad Nacional de Cordoba we evaluated the mechanism of molecular iodine catalysed transformation of alcohols using DFT calculation methodology.

In collaboration with Faculty of Biotechnology UL and company Alkemika we have developed compounds from the family of beta keto esters derivatives as the new type of precursors for biosynthesis of tetracycline. Special attention was paid to the derivatives bearing at least one fluorine atom into target molecules.

### Some outstanding publications in the past year

- 1. G. Šekularac, I. Milošev, Corrosion of aluminium alloy AlSi7Mg0.3 in artificial sea water with added sodium sulphide, Corros. Sci. 144 (2018), 54-73
- I. Milošev, G.S. Frankel, Review–Conversion coatings based on zirconium and/or titanium, J. Electrochem. Soc. 165 (2018), C127-C144
- T. Matsushima, A. Kokalj, Angle-resolved desorption and removal of surface nitrogen in deNOx, Surf. Sci. Rep. 73 (2018) 191-212
- J.J. Corral-Pérez, A. Bansode, C.S. Praveen, A. Kokalj, H. Reymond, A. Comas-Vives, J. VandeVondele, C. Copéret, P.R. von Rohr, A. Urakawa, Decisive Role of Perimeter Sites in Silica-Supported Ag Nanoparticles in Selective Hydrogenation of CO<sub>2</sub> to Methyl Formate in the Presence of Methanol, J. Am. Chem. Soc. 140 (2018) 13884-13891
- K. Čebular, S. Stavber. Molecular iodine as a mild catalyst for cross-coupling of alkenes and alcohols, Pure Appl. Chem. 90 (2018) 377-38

### Awards and Appointments

- 1. Damir Hamulić, Ingrid Milošev, Peter Rodič, Dolores Zimerl: Award for best invention/innovation with the commercial potential at 11. ITTC in 2018.
- 2. Urša Tiringer, Gavrilo Šekularac: "Young Author's EFC Poster Prize EUROCORR 2018".
- 3. Ingrid Milošev, Peter Rodič: Krka Prize for secondary school research papers award for mentorship.

### Organization of conferences, congresses and meetings

- 1. CorrTalk: Workshop on integrative approaches to corrosion research, Ljubljana, Slovenia, 11. 13. 6. 2018
- How to Conduct a Successful PhD: MAMI (Magnetism and Microhydrodynamics, H2020 MSCA-ITN-2017-766007), Ljubljana, Slovenia, 5. - 7. 12. 2018
- 3. Ingrid Milošev, Peter Rodič: Silver Award at the 52th Meeting of young researchers Slovenia award for mentorship.

### INTERNATIONAL PROJECTS

- COST MP1402 HERALD; Hooking together European Research in Atomic Layer Deposition
   Deposition
  - Dr. Peter Rodič Cost Association Aisbl
- 2. COST CA17126: Towards Understanding and Modelling Intense Electronic Excitation

Asst. Prof. Anton Kokalj	
Cost Association Aisbl	
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- H2020 STEM4youth; Promotion of STEM Education by Key Scientific Challenges and their Impact on Our Life and Career Perspectives Dr. Peter Rodič
- European Commission
- H2020 mCBEEs; Advanced Integrative Solutions to Corrosion Problems Beyond Micro-Scale: Towards Long-Term Durability of Miniaturized Biomedical, Electronic and Energy Systems

#### Prof. Ingrid Milošev

European Commission

- 5. H2020 MAMI; Magnetics and Microhydrodynamics From Guided Transport to Delivery
  - Prof. Ingrid Milošev
- European Commission 6. INCOR: INterfaces relevant for CORrosion and its inhibition
- Prof. Ingrid Milošev Slovenian Research Agency
- 7. Fundamental Insights Into Fuel Cell Electrocatalysis Combination of Modelling and Experiment

Asst. Prof. Anton Kokalj Slovenian Research Agency

### RESEARCH PROGRAMS

 Chemistry for sustainable development Dr. Peter Rodič

### VISITORS FROM ABROAD

- prof. dr. Hadi Behzadi, Faculty of Chemistry, Kharazmi University, Tehran, Iran, 24. 7. - 15. 9. 2018
- dr. Fatah Chiter, Chemie ParisTech, PSL University, CNRS, Institut de Recherche de Chimie Paris, France, 22. 10. - 31. 10. 2018

### STAFF

#### Researchers

- 1. Asst. Prof. Anton Kokalj
- 2. Dr. Antonija Lesar, retired 01.12.18
- 3. Dr. Matic Lozinšek, left 01.07.18
- 4. Prof. Ingrid Milošev, Head
- 5. Prof. Stojan Stavber Postdoctoral associates
- 6 Dr Peter Rodič
- 7. Dr. Urša Tiringer
- Postgraduates
- 8. Klara Čebular, B. Sc.

 Advanced materials for low-carbon and sustainable society Prof. Ingrid Milošev

### R & D GRANTS AND CONTRACTS

- Modulation of polyketid synthase complex involved in early and late stages of tetracycline biosynthesis Prof. Stojan Stavber
- Multidisciplinary approach towards development of a novel multifunctional heterogeneous catalyst for efficient conversion of H2 and CO2 gas mixtures into fuel additives and surrogates Asst. Prof. Anton Kokalj
- COR\_ID: Design of corrosion resistant coatings targeted for versatile applications Prof. Ingrid Milošev
- Ministry of Education, Science and Sport
  COIN DESC: IntegratedComputational Materials Engineering entitled Corrosion inhibition and dealloying descriptors
  Asst. Prof. Anton Kokalj
  Ministry of Education, Science and Sport
- prof. dr. Igor Pašti, Faculty of physical chemistry, University of Belgrade, Belgrade, Serbia, 27. 11. - 3. 12. 2018
- dr. Dominique Costa, Chemie ParisTech, PSL University, CNRS, Institut de Recherche de Chimie Paris, Paris, France, 18. 12. - 21. 12. 2018
- 9. Matjaž Dlouhy, B. Sc.
- 10. Dunja Gustinčič, B. Sc., left 01.07.18
- 11. Damir Hamulić, B. Sc.
- 12. Nikolina Lešić, B. Sc.
- 13. Matic Poberžnik, B. Sc.
- 14. Ivan Spajić, B. Sc.
- 15. Gavrilo Šekularac, B. Sc. Technical officers
- 16. Barbara Kapun, B. Sc.
- 17. Dolores Zimerl, B. Sc.

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### **ORIGINAL ARTICLE**

- Vesna Levašič, Ingrid Milošev, Vesna Zadnik, "Risk of cancer after primary total hip replacement: the influence of bearings, cementation and the material of the stem", *Acta orthopaedica*, 2018, 89, 2, 234-239.
- Gavrilo Šekularac, Ingrid Milošev, "Corrosion of aluminium alloy AlSi7Mg0.3 in artificial sea water with added sodium sulphide", *Corrosion science*, 2018, 144, 54-73.
- 3. Žiga Zupanek, Melita Tramšek, Anton Kokalj, Gašper Tavčar, "Reactivity of VOF<sub>3</sub> with N-heterocyclic carbene and imidazolium fluoride: analysis of ligand-VOF<sub>3</sub> bonding with evidence of a minute  $\pi$  back-donation of fluoride", *Inorganic chemistry*, 2018, **57**, 21, 13866-13879.
- 4. Matic Poberžnik, Dominique Costa, Anne Hemeryck, Anton Kokalj, "Insight into the bonding of silanols to oxidized aluminum surfaces", *The journal of physical chemistry. C, Nanomaterials and interfaces*, 2018, **122**, 17, 9417-9431.
- 5. Urša Tiringer, Ingrid Milošev, Alicia Dúran, Yolanda Castro, "Hybrid solgel coatings based on GPTMS/TEOS containing colloidal  $SiO_2$  and cerium nitrate for increasing corrosion protection of aluminium alloy 7075-T6", *Journal of sol-gel science and technology*, 2018, **85**, 3, 546-557.

- 6. Juan José Corral-Pérez *et al.* (11 authors), "Decisive roles of perimeter sites in silica-supported Ag nanoparticles in selective hydrogenation of CO<sub>2</sub> to methyl formate in the presence of methanol", *Journal of the American Chemical Society: JACS*, 2018, **140**, 42, 13884-13891.
- 7. Urša Tiringer, Alicia Dúran, Yolanda Castro, Ingrid Milošev, "Selfhealing effect of hybrid sol-gel coatings based on GPTMS, TEOS, SiO<sub>2</sub> nanoparticles and Ce(NO<sub>3</sub>)<sub>3</sub> applied on aluminum alloy 7075-T6", *Journal of the Electrochemical Society*, 2018, **165**, 5, c213-c225.
- 8. Peter Rodič, Jozefina Katić, Dorota Korte, Paula M. Desimone, Mladen Franko, Silvia Ceré, Mirjana Metikoš-Huković, Ingrid Milošev, "The effect of cerium ions on the structure, porosity and electrochemical properties of Si/Zr-based hybrid sol-gel coatings deposited on aluminum", *Metals*, 2018, 8, 4, 248.
- 9. Dunja Gustinčič, Anton Kokalj, "DFT study of azole corrosion inhibitors on  $Cu_2O$  model of oxidized copper surfaces. I. Molecule-surface and Cl-surface bonding", *Metals*, 2018, **8**, 5, 310.
- Dunja Gustinčič, Anton Kokalj, "DFT study of azole corrosion inhibitors on Cu<sub>2</sub>O model of oxidized copper surfaces. II. Lateral interactions and thermodynamic stability", *Metals*, 2018, 8, 5, 311.
- 11. Klara Čebular, Bojan Đ. Božić, Stojan Stavber, "Esterification of aryl/alkyl acids catalysed by N-bromosuccinimide under mild reaction conditions", *Molecules*, 2018, **23**, 9, 2235.

- 12. Peter Rodič, Ingrid Milošev, Maria Lekka, Francesco Andreatta, Lorenzo Fedrizzi, "Corrosion behaviour and chemical stability of transparent hybrid sol-gel coatings deposited on aluminium in acidic and alkaline solutions", *Progress in organic coatings*, 2018, **124**, 286-295.
- 13. Klara Čebular, Stojan Stavber, "Molecular iodine as a mild catalyst for cross-coupling of alkenes and alcohols", *Pure and applied chemistry*, 2018, **90**, 2, 377-386.
- 14. Damir Hamulić, Ingrid Milošev, Dirk Lützenkirchen-Hecht, "The effect of the deposition conditions on the structure, composition and morphology of electrodeposited cobalt materials", *Thin solid films*, 2018, 667, 11-20.
- 15. Gabriela L. Borovsky, Stojan Stavber, Kenneth K. Laali, "Iodine activation of alcohols: a computational study", *Topics in catalysis*, 2018, **61**, 7/8, 636-642.

### **REVIEW ARTICLE**

- 1. Njomza Ajvazi, Stojan Stavber, "Alcohols in direct carbon-carbon and carbon-heteroatom bond-forming reactions: recent advances", *ARKIVOC*, 2018, ii, 288-329.
- Ingrid Milošev, Gerald S. Frankel, "Review-conversion coatings based on zirconium and/or titanium", *Journal of the Electrochemical Society*, 2018, 165, 3, c127-c144.
- 3. Tatsuo Matsushima, Anton Kokalj, "Angle-resolved desorption and removal of surface nitrogen in deNOx", *Surface Science Reports*, 2018, **73**, 5, 191-212.

### PUBLISHED CONFERENCE CONTRIBUTION

1. Matic Poberžnik, Anton Kokalj, "Lateral interactions between electronegative adatoms on metallic surfaces", In: Natalia V. Skorodumova (ed.), Igor A. Pašti (ed.), Biljana Šljukić Paunković (ed.), *Book of abstracts*, 3rd International Meeting on Materials Science for Energy Related Applications, [within] Physical Chemistry 2018, 14th International Conference on Fundamental and Applied Aspects of Physical Chemistry, September 25-26, 2018, Belgrade, Serbia, 2018, 80-81.

2. Anton Kokalj, Juan José Corral-Pérez, Atul Bansode, C. S. Praven, Helena Reymond, Aleix Comas-Vives, J. Vande Vondele, Christophe Copéret, Philipp Rudolf von Rohr, Atsushi Urakawa, "Unique reactivity of silver on silica CO<sub>2</sub> hydrogenation to formates and subsequent esterification with methanol to methyl formate", In: Natalia V. Skorodumova (ed.), Igor A. Pašti (ed.), Biljana Šljukić Paunković (ed.), *Book of abstracts*, 3rd International Meeting on Materials Science for Energy Related Applications, [within] Physical Chemistry 2018, 14th International Conference on Fundamental and Applied Aspects of Physical Chemistry, September 25-26, 2018, Belgrade, Serbia, 2018, 55-56.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

- Tatsuo Matsushima, Anton Kokalj, "An approach to structure-sensitive desorption dynamics", In: Klaus Wandelt (ed.), *Encyclopedia of interfacial chemistry: surface science and electrochemistry*, 2018, 31-39.
- 2. Anton Kokalj, Dominique Costa, "Molecular Modeling of corrosion inhibitors", In: Klaus Wandelt (ed.), *Encyclopedia of interfacial chemistry: surface science and electrochemistry*, 2018, 332-345.

### MENTORING

- 1. Urša Tiringer, *Hybrid sol-gel coatings with barrier and self-healing properties for corrosion protection of aluminum alloys:* doctoral dissertation, Ljubljana, 2018 (mentor Ingrid Milošev).
- 2. Barbara Volarič, *Conversion coatings of lanthanoide salts for the protection of aluminium alloys:* doctoral dissertation, Ljubljana, 2018 (mentor Ingrid Milošev; co-mentor Miran Gaberšček).

## **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 ceramics, we continued our research of sodium potassium niobate (K<sub>a</sub>, Na<sub>a</sub>, NbO<sub>a</sub>, KNN) based materials, which could replace the efficient lead-based piezoelectrics. To reduce or to avoid chemical heterogeneities, often encountered in the conventional solid-state synthesis of complex perovskites, the mechanochemical activation of reagent particles was introduced in the processing of the (K,Na,Li)(Nb,Ta) O,-CaZrO, based ceramic. Partial amorphisation of the reagents contributed to a much lower final temperature of Head:



the solid-state reaction, the ceramic exhibited a higher level of chemical homogeneity and enhanced ferro- and Prof. Barbara Malič piezoelectric properties in comparison to conventionally processed material.

The coupling between antiferromagnetic and ferroelectric/ferroelastic domain switching in polycrystalline BiFeO<sub>2</sub> has been studied for the first time. Using in-situ neutron-diffraction analysis we directly observed the antiferromagnetic domain switching induced by non-180° ferroelectric/ferroelastic domain texturing during electric field application. Along with the orientation dependence of this coupled switching, these data represent the first step towards understanding and manipulating the antiferromagnetic order using the electric field in polycrystalline BiFeO<sub>2</sub>.

In collaboration with colleagues from the School of Materials Science and Engineering, University of New South Wales, Sydney, Australia, the Swiss Federal Institute of Technology in Lausanne, Switzerland and ESRF-The European Synchrotron, Grenoble, France, we studied an unusual strain behaviour of individual grains inside a polycrystalline matrix of bismuth ferrite. In contrast to the frequency behaviour of the strain arising from domain-wall displacements, the lattice strain showed an unexpected decreasing magnitude with decreasing field frequency. This strain decoupling was explained by analytical modelling, confirming the key role of the anisotropy in the electrical conductivity caused by the different orientation of conductive domain walls in different grains within the polycrystalline matrix. (Figure 1)

In-situ synchrotron XRD analysis was used to gain an insight into the mechanisms of an electric-field-induced phase transformation in samarium-doped BiFeO, ceramics, which are believed to play the key role in the electromechanical response of this class of multiferroic materials. The results revealed two transformation pathways related to a reversible antiferroelectric-to-ferroelectric and irreversible paraelectric-to-ferroelectric phase transformations with slow dynamics (a time constant of minutes). The findings point to texturing and the elimination of the paraelectric phase as the origin of the enhanced electromechanical response.

We studied the influence of cobalt doping on the electrical conductivity and domain-switching behaviour of rare-earth-modified bismuth ferrite (Bi<sub>0.01</sub>Dy<sub>0.00</sub>)FeO<sub>3</sub> ceramics. Undoped samples showed exceedingly large leakage currents under switching field conditions that were successfully suppressed by cobalt doping. We tentatively attributed this effect to the binding of the Co-dopant into the defect complexes which suppresses the

### Projects INTcerSEN and PiezoMEMS have been awarded the title of "Success story M-ERA.NET"

M-ERA.NET is an EU-funded network with the mission to support and increase the coordination of European research and innovation programmes and related funding in materials science and engineering. Over the last three years, twenty M-ERA.NET European projects have been awarded the title of "Success story M-ERA.NET". At the Electronic Ceramics Department we have participated in two projects that last year received the "Success story" titles.

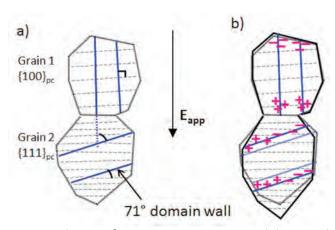


Figure 1: Schematic of two representative grains in poled  $BiFeO_x$  a) Illustration of 71° domain walls in two grains of different orientations forming different angles with respect to the electric-field axis  $E_{abb}$ , b) Charge re-distribution in the two grains upon the application of the electric field  $E_{app}$  arising due to the different orientation of the conductive domain walls with respect to  $E_{app}$ . This charge re-distribution and the corresponding change in internal fields are responsible for the peculiar frequency dependence and decoupling of strain mechanisms in BiFeO<sub>x</sub>

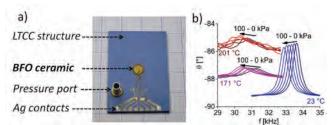


Figure 2: a) Photograph of the pressure sensor with an integrated bulk BiFeO<sub>3</sub> piezoelectric actuator. b) Phase angle  $\theta$  as a function of frequency for the sensor measured at three different temperatures. At each temperature, the measurement was performed by varying the differential pressures (from 0 kPa to 100 kPa). The arrows indicate curves for increasing differential pressure. The measurements confirmed a pressure sensitivity, i.e., resonance frequency shift of the sensor per unit of pressure, of -8.7 Hz/kPa up to 171 °C.

charge de-trapping at high electric fields, effectively reducing the high-field leakage current by an order of magnitude with respect to undoped ceramics.

Later, we constructed a ceramic pressure sensor from the low-temperature co-fired ceramic (LTCC) with an integrated bulk  $BiFeO_3$  piezoelectric actuator that could operate at elevated temperatures. In order to construct a sensor with a suitable pressure sensitivity, numerical simulations were used to define the optimum construction dimensions. The sensor's functionality was proven to be sufficient up to 171 °C. (*Figure 2*)

In collaboration with the Advanced Materials Department we studied the piezoelectric and ferroelectric properties of micrometre- to nanometresized Ba<sub>1x</sub>Sr<sub>x</sub>TiO<sub>3</sub> plates using piezoresponse force microscopy (PFM). We found that Ba<sub>1x</sub>Sr<sub>x</sub>TiO<sub>3</sub> plates with  $0 \le x \le 0.175$  exhibited ferroelectric and piezoelectric characteristics, while the plates with a larger amount of strontium were non-piezoelectric. The study opens up new possibilities for the use of such plates in the field of miniature piezoelectric sensors.

Research on lead-based ferroic materials continued with  $1-xPb(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3$  (PMN-100xPT) ceramics, processed by mechanochemical synthesis and sintering. The PMN-10PT relaxor ceramic is known for its high electrocaloric properties, yet it is quite challenging to obtain a phase-pure material. Adding the PbTiO\_3 seeds to remaining oxide constituents prior to mechanochemical activation reduced the milling time needed to achieve a pure perovskite PMN-10PT by about a half. By following the perovskite crystallization process by X-ray diffraction (XRD) and transmission electron microscopy (TEM) analyses, we also demonstrated that a second, metastable, pyrochlore phase is taking part in the perovskite formation.

We further investigated a broad range of PMN-100xPT compositions, from ergodic relaxor to relaxor ferroelectric, their structure and their response to external fields at various length-scales using in-situ XRD, ex-situ TEM and

MIDEM conference - Between the 3<sup>rd</sup> and 5<sup>th</sup> of October 2018, the 54<sup>th</sup> International Conference on Microelectronics, Devices and Materials with the Workshop on Sensors and Transducers was held at the Jožef Stefan Institute. The conference was chaired by Dr. Tadej Rojac and Dr. Hana Uršič and organized by the MIDEM society and SRIP Factories of the Future. Participants from seven European countries, North America and China contributed to the international scientific discussion. PFM. From the observed changes in the crystal and domain structures, combined with macroscopic measurements of the responses to electric fields, we were able to determine the main contributions to the overall properties. These were shown to obviously differ in monoclinic compositions with the nanodomain texture (0.2 < x < 0.33) from the tetragonal compositions (x>0.35) with the lamellar domains and the more 'classic' ferroelectric behaviour. The results point out the significant extrinsic effects of the monoclinic nanodomains and their movement to the high electromechanical responses in relaxor ferroelectric ceramics. (*Figure 3*)

In collaboration with colleagues from North Carolina State University, USA, electric-field-induced changes in the PMN-30PT composition were followed by in-situ high-energy XRD and pair-distribution function (PDF)

analyses. These measurements of the long-range and local scale responses, respectively, revealed that a field-induced polarization occurs, which was shown for the first time in polycrystalline ferroelectrics.

In collaboration with colleagues from the Technical University Darmstadt, Germany, we aimed at exploring the possibility of optimizing the **electrocaloric** (EC) response with defect engineering. The impact of defects on the EC response was studied in  $Pb(Zr,Ti)O_3$  (PZT) ceramics doped with acceptor and donor dopants. The highest

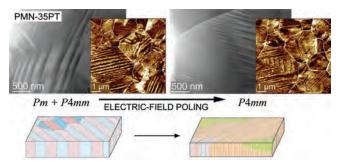


Figure 3: Evolution of the domain structure of PMN-PT ceramics at the morphotropic phase boundary with ex-situ applied electric field. TEM micrographs and PFM images (and the corresponding sketch) show the reorientation and densification of the lamellar domain walls, which was simultaneous with a phase change from tetragonal and monoclinic coexisting symmetries to a more tetragonal one.

EC cooling was observed in acceptor-doped PZT when the electric field was applied parallel to the aligned defect complexes. The origin of this largest EC response was attributed to the reduced hysteresis losses and the associated self-heating effects, which seem to play a key role in the EC response of PZT.

We proceeded with an investigation of the **multicaloric effect** in  $Pb(Fe_{1/2}Nb_{1/2})O_3$ -based ceramics. The ceramics were prepared by the mechanochemical activation of constituent oxides, followed by a thermal treatment. We investigated the influence of manganese, lithium and cobalt doping on the functional properties of polycrystalline  $Pb(Fe_{1/2}Nb_{1/2})O_3$ .

In collaboration with the Luxembourg Institute of Science and Technology (LIST) we continued the research of solution-derived **tuneable ferroelectric (Ba,Sr)TiO<sub>3</sub> thin films**. The dielectric permittivity, losses and voltage tunability in the microwave range (~10 GHz) of the perovskite films with a columnar microstructure are effectively tailored by changing the Ba/Sr molar ratio and/or by manganese doping for a given microwave component. Together with colleagues from LIST and the Faculty of Elec-

trical Engineering, University of Ljubljana, we designed and fabricated a frequency-agile planar antenna based on a (Ba,Sr)TiO<sub>3</sub> thin-film varactor.

In collaboration with the Advanced Materials Department we studied the local piezoelectric and ferroelectric properties of  $0.66Pb(Mg_{1/3}Nb_{2/3})$  $O_3-0.33PbTiO_3$  thin films prepared by pulsed-laser deposition. Using piezoresponse force microscopy we confirmed the effective poling and ferroelectric domain switching in these films. The local piezoelectric response  $(d_{33}^{-local})$  of the surface structure reached values as high as 140 pm/V, while the average piezoelectric value was 28 pm/V. The results of this study offer an excellent starting point for the preparation of functional thin films for  $d_{32}$ -mode energy harvesters.

We investigated the **electrophoretic deposition** of **thick-films** of environmentally benign piezoelectrics based on  $K_{0.5}Na_{0.5}NbO_3$  on metallized corundum substrates for energy-harvesting applications in collaboration with researchers from François-Rabelais University, Tours, France. After sintering at 1110 °C the ~ 20-µm-thick films with a relative density of 82 % exhibited promising electromechanical properties; a piezoelectric coefficient d<sub>z2</sub> of 80 pC / N and an average thickness coupling factor k, of 40 %.

We proceeded with microstructural investigations of a few- $\mu$ m to several-tens-of- $\mu$ m thick BiFeO<sub>3</sub> films deposited on platinized Al2O3. The thick-films were prepared by the screen printing method.

Using screen printing we prepared test structures for single-chamber solid-oxide fuel cells. The  $(La,Sr)MnO_3$  cathode, Ni anodes, and a mesh of platinum were screen printed on a crystal of  $ZrO_2$  stabilized with  $Y_2O_3$  (YSZ). Colleagues from the Synchrotron Elettra, Trieste, Italy, investigated the chemical state of the constituents of a fuel cell with X-ray photoelectron spectroscopy with a sub-micrometre resolution and at a pressure of ~1 bar. Understanding the chemical state of the electrode materials under operating conditions is of paramount importance for improving the energy efficiency of single-chamber fuel cells.

We have started with the **aerosol deposition** of functional-oxide thick films. The aerosol deposition system is a part of the **Laboratory for the ultracool preparation of complex oxides**, in short ULTRACOOL, for which financial support was granted by the **Director's Fund 2017** project. Current research is focused on the optimization of processing parameters for the preparation of functional 0.9Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-0.1PbTiO<sub>3</sub> thick films on metal and ceramic substrates. (*Figure 4*)

We deposited **conductive oxide** LaNiO<sub>3</sub> (LNO) electrodes on top of ferroelectric Pb(Zr,Ti)O<sub>3</sub> (PZT) thin films on platinized silicon substrates using the technology of **inkjet printing**. We designed an LNO ink based on a combination of solvents with a range of viscosities, surface tensions and boiling points, which enabled us to reproducibly pattern LNO layers with lateral dimensions of a few 100  $\mu$ m and a uniform thickness of a few 10 nm. The functional properties of thin-film capacitors with inkjet-printed

LNO top-electrodes outperform those with sputtered gold top-electrodes (~40% higher dielectric permittivity, improved fatigue properties), which is probably related to the effective compensation of oxygen vacancies by the oxide electrode, thinner depletion regions at the LNO-PZT interface, and a lower concentration of charged defects due to the processing. The research was performed in collaboration with colleagues from the Departments of Condensed Matter Physics, Thin Films and Surfaces, and Surface Engineering and Optoelectronics. (Figure 5).

LTCC (Low Temperature Co-Fired Ceramics) and thick-film materials and processes have been investigated for the design and fabrication of three-dimensional ceramic structures for the packaging of microelectronic components and systems, so-called System in Package (SiP). An advantage of the LTCC is the heterogeneous integration of various electronic and other components, and at the same time high-quality protection in demanding environments. In cooperation with CoE NAMASTE, HIPOT-RR and KEKO Equipment, we successfully developed ceramic structures with integrated sensors and microfluidic elements for the packaging of microelectromechanical systems (MEMS). The results are useful in the designing and manufacturing of Smart Systems in Package, especially in emerging projects.



Figure 4: a) Laboratory for the ultracool preparation of complex oxides, in short ULTRACOOL (Director's Council 2017). The image shows a device for the aerosol deposition of thick films that is based on accelerated particles heating the substrate and forming a dense thick film at room temperature. b) Photograph of a thick film prepared in the ULTRACOOL lab.

Our colleague Dr. Tadej Rojac received two awards: i) The Young Investigator Award of the IEEE Ultrasonics, Ferroelectrics and Frequency Control Society for his pioneering work in the processing of chemically complex ferroelectric ceramics and ii) the Zois Recognition for significant achievements in the research of the synthesis and characterization of high-temperature piezoelectric ceramics based on bismuth ferrite.

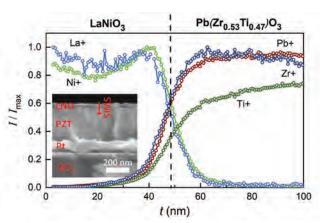


Figure 5: ToF SIMS analysis of the chemical composition of a thin-film capacitor LaNiO<sub>3</sub>/Pb(Zr<sub>0.53</sub>Ti<sub>0.47</sub>)O<sub>3</sub>(PZT)/Pt on a SiO<sub>2</sub>/Si substrate in the direction marked by an arrow. Inset: scanning electron micrograph of the cross-section of the capacitor.

### Some outstanding publications in the past year

- Liu, Lisha, Rojac, Tadej, Damjanović, Dragan, Di Michiel, Marco, Daniels, John E. Frequency-dependent decoupling of domain-wall motion and lattice strain in bismuth ferrite. Nature communications, ISSN 2041-1723, 2018, vol. 9, pp. 4928-1-4928-10, doi: 10.1038/s41467-018-07363-y. [COBISS.SI-ID 31884583]
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- Matavž, Aleksander, Kovač, Janez, Čekada, Miha, Malič, Barbara, Bobnar, Vid. Enhanced electrical response in ferroelectric thin film capacitors with inkjet-printed LaNiO<sub>3</sub> electrodes. Applied physics letters, ISSN 0003-6951. [Print ed.], 2018, vol. 113, no. 1, pp. 012904-1-012904-4, doi: 10.1063/1.5037027. [COBISS.SI-ID 31521063]
- Walker, Julian, Bayer, Thorsten J. M., Makarovič, Maja, Kos, Tomaž, Trolier-Mckinstry, Susan, Malič, Barbara, Rojac, Tadej.
   Cobalt doping to influence the electrical conductivity of (Bi<sub>0.91</sub>Dy<sub>0.09</sub>)FeO<sub>3</sub> ceramics. Materials letters, ISSN 0167-577X. [Print ed.], 2018, vol. 225, pp. 126-129, doi: 10.1016/j.matlet.2018.04.125. [COBISS. SI-ID 31357479]

### Awards and Appointments

- 1. Tadej Rojac: Young investigator award for his pioneering work in processing of chemically complex ferroelectric ceramics, IEEE Ultrasonics Ferroelectrics and Frequency Control Society
- 2. Tadej Rojac: Zois Award for significant achievements in research of the synthesis and characterization of high-temperature piezoelectric ceramics based on bismuth ferrite, Government of the Republic of Slovenia

### Organization of Conferences, Congresses and Meetings

1. MIDEM 2018: 54<sup>th</sup> International Conference on Microelectronics, Devices and Materials with the Workshop on Sensors and Transducers, Ljubljana, October 3 – 5, 2018

### Patents granted

- Irena Ramšak, Marija Razpotnik, Katja Makovšek, Danjela Kuščer, Silvo Drnovšek, Janez Holc, Production method of steatite ceramics with improved electrical properties, EP3230232 (B1), European Patent Office, 15. 08. 2018.
- 2. Irena Ramšak, Marija Razpotnik, Janez Holc, Danjela Kuščer, Method for producing non-alkaline steatite ceramics with improved electrical properties, EP3233755 (B1), European Patent Office, 10. 10. 2018.
- Barbara Malič, Hana Uršič, Marija Kosec, Silvo Drnovšek, Jena Cilenšek, Zdravko Kutnjak, Brigita Rožič, Uroš Flisar, Andrej Kitanovski, Marko Ožbolt, Uroš Plaznik, Alojz Poredoš, Urban Tomc, Jaka Tušek, Method for electrocaloric energy conversion, US9915446 (B2), US Patent and Trademark Office, 13. 03. 2018.

### INTERNATIONAL PROJECTS

- 1. COST MP1308; Towards Oxide Based Electronics (TO-BE) Asst. Prof. Hana Uršič Nemevšek
- COST Office
- 2. Minor Services Foreign Customers Prof. Barbara Malič
- 3. Advanced Electronic Ceramics for the Sustainable, Efficient and Safe Use of Energy Prof. Barbara Malič
- Slovenian Research Agency 4. Domain Structure of Complex Oxides
- Asst. Prof. Hana Uršič Nemevšek Slovenian Research Agency
- Local Structure in Relaxor Ferroelectrics The Key to Understanding their Functional Properties Prof. Andreja Benčan Golob
- Slovenian Research Agency

- Environment Friendly Ferroelectric Materials in Bulk and Thin-Film Forms and Low-Temperature Processing Thereof Prof. Barbara Malič
- Slovenian Research AgencyProcessing of Piezoelectric Thick Films by Aerosol Deposition Technique Asst. Prof. Hana Uršič Nemevšek
- Slovenian Research Agency
- Novel Hardening Mechanisms in Lead-Free Piezoceramics Prof. Tadej Rojac Slovanian Research Agency.
- Slovenian Research Agency 9. Cold Sintering of Complex Oxide Materials
- Cold Sintering of Complex Oxide Dr. Mojca Otoničar Slovenian Research Agency

### RESEARCH PROGRAM

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

### R & D GRANTS AND CONTRACTS

- Photovoltaic cell and modul inhomogenity analysis and performace monitoring in power plants through lifetime Prof. Barbara Malič
- Multifunctional materials for actuator and cooling devices Prof. Tadej Rojac
- Multicaloric cooling
- Asst. Prof. Hana Uršič Nemevšek
- 4. Advanced electrocaloric energy conversion
- Prof. Barbara Malič
- 5. Domain engineered ferroelectric ceramic layer elements for efficient energy harvesting

### VISITORS FROM ABROAD

- Hugo Mercier, François Rabelais University of Tours, Tours, France, January 22 February 17, 2018
- Marija Lovreković, Bjelovar University of Applied Sciences, Bjelovar, Croatia, February 19 – April 20, 2018
- 3. Dr. Julian Walker, Pennsylvania State University, Pennsylvania, USA, March 5 9, 2018
- 4. Dumitru Rotari, University of Petrosani, Petrosani, Romania, March 5 May 25, 2018
- 5. Mirela Goncear, University of Petrosani, Petrosani, Romania, March 5 May 25, 2018
- Alan Mutka, Bjelovar University of Applied Sciences, Bjelovar, Croatia, March 15, 2018
   Ivan Marušić, Bjelovar University of Applied Sciences, Bjelovar, Croatia, March 20 -
- 23, 2018 8. Ivan Sekovanić, Bielovar University of Applied Sciences, Bielovar, Croatia, March 20 -
- Ivan Sekovanić, Bjelovar University of Applied Sciences, Bjelovar, Croatia, March 20 23, 2018
- 9. Ivana Jurković, Bjelovar University of Applied Sciences, Bjelovar, Croatia, March 20 23, 2018
- Paul Lechesne, Université François-Rabelais Tours, Tours, France, April 3 June 22, 2018
- Grégorie Levavasseur, Université François-Rabelais Tours, Tours, France, April 3 -June 22, 2018
- 12. Hanae Azeroual, University of Limoges, Limoges, France, April 9 July 15, 2018
- 13. Prof. Kenji Uchino, Pennsylvania State University, Pennsylvania, USA, May 10 17, 2018
- 14. Rachel Sherbondy, Colorado School of Mines, Golden, Colorado, USA, May 21 -July 27, 2018
- Toni Fak, Bjelovar University of Applied Sciences, Bjelovar, Croatia, July 2 October 10, 2018
- Antonio Lisičak, Bjelovar University of Applied Sciences, Bjelovar, Croatia, July 2 December 31, 2018
- Hicran Arslan, Yildiz Technical University Istanbul, Istanbul, Turkey, July 16 October 14, 2018
- Dr. Pedro Braga Groszewicz, Eduard-Zint Institut Darmstadt, Darmstadt, Germany, September 6, 2018

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- 1. Prof. Andreja Benčan Golob
- 2. Prof. Goran Dražić\*
- 3. Asst. Prof. Danjela Kuščer Hrovatin
- 4. Prof. Barbara Malič, Head
- 5. Dr. Mojca Otoničar
- 6. Prof. Tadej Rojac
- 7. Asst. Prof. Hana Uršič Nemevšek
- Postdoctoral associates
- 8. Dr. Mirela Dragomir, left 01.05.18
- 9. Dr. Kostja Makarovič\*
- 10. Dr. Kristian Radan
- 11. Dr. Tanja Vrabelj
- 12. Dr. Marko Vrabelj, left 14.05.18 Postgraduates
- 13. Andraž Bradeško, B. Sc.

- and energy conversion applications Prof. Barbara Malič
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Barbara Malič
- Ministry of Economic Development and Technology
- Inkjet Printing of PZT Test Structures and Piezoelectric Characterization of Thin Films Double-Beam Laser Interferometer Measurement
- Prof. Barbara Malič
  Stay of Maja Makarovič in Trondheim Interactions between Charged Defects and Domain Walls in Lead-Free BiFeO3
- Maja Makarovič 9. Stay of Mojca Otoničar in Lausanne - Pursuing the Origin of the Large Irreversible Contribution to Piezoelectric Responsein the Monoclinic Phases of Pb(Mg1/3Nb2/3) 03-xPbTiO3 Ceramics Dr. Mojca Otoničar
- 10. Laboratory Measurements
- Asst. Prof. Hana Uršič Nemevšek
- Sample Preparations Prof. Andreja Benčan Golob
- 19. Dr. Marko Vrabelj, EPCOS OHG, Deutschlandsberg, Germany, September 11 14, 2018
- Matija Buljan, Bjelovar University of Applied Sciences, Bjelovar, Croatia, September 24 - December 23, 2018
- Antun Čordaš, Bjelovar University of Applied Sciences, Bjelovar, Croatia, September 24 - December 23, 2018
- Prof. Dragan Damjanovic, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland, September 30 – October 4, 2018
- Prof. Franck Levassort, Université François-Rabelais Tours, Tours, France, October 3 5, 2018
- Dr. Alexander Martin, Friedriech-Alexander Universität Erlangen-Nuernberg, Nuernberg, Germany, October 7 – 20, 2018
- 25. Prof. Angus I. Kingon, Brown University, Providence, USA, October 5, 2018
- Nicole Bartek, Universität Druisburg-Essen, Essen, Germany, October 8 November 2, 2018
- Yuji Matshushita, Osaka Prefecture University, Osaka, Japan, October 10 December 31, 2018
- Kevin Riess, Friedriech-Alexander Universität Erlangen-Nuernberg, Nuernberg, Germany, November 5 – 23, 2018
- Dr. Neamul Hayet, Friedriech-Alexander Universität Erlangen-Nuernberg, Nuernberg, Germany, November 5 – 23, 2018
- 30. Dr. Denis Orosel, EPCOS OHG, Deutschlandsberg, Germany, November 6, 2018
- 31. Dr. Marko Vrabelj, EPCOS OHG, Deutschlandsberg, Germany, November 12 16, 2018
- Dr. Jurij Koruza, Technische Universität Darmstadt, Darmstadt, Germany, November 19 – 30, 2018
- Marion Hofling, Technische Universität Darmstadt, Darmstadt, Germany, November 19 – 30, 2018
- 34. Milan Baričević, University of Bjelovar, Bjelovar, Croatia, December 17 31, 2018
- Prof. Jürgen Rödel, Technische Universität Darmstadt, Darmstadt, Germany, December 17 – 19, 2018
- 14. Oana Andreea Condurache, B. Sc.
- 15. Lovro Fulanović, B. Sc.
- 16. Maja Makarovič, B. Sc.
- 17. Uroš Prah, B. Sc.
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   Silvo Drnovšek, B. Sc.
- 20. Shvo Dinovsek, B. Sc. 21. Brigita Kmet, B. Sc.
- Technical and administrative staff
- 22. Tamara Matevc, B. Sc., 06.10.18, transferred to Department E6
- Tina Ručigaj Korošec, B. Sc., OO.1
- 25. Thia Rueigaj Rotosee, D. Se.

Note:

\* part-time JSI member

 25. Froi. Franck Levassort, Universite Franço 2018
 24. Dr. Alexander Martin, Friedriech-Alexand Nucerbarg, Correspondent October 7, 20, 201

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- 2. Mario Špadina, Simon Gourdin-Bertin, Goran Dražić, Atiđa Selmani, Jean-François Dufrêche, Klemen Bohinc, "Charge properties of TiO  $_2$  nanotubes in NaNO  $_3$  aqueous solution", *ACS applied materials & interfaces*, 2018, **10**, 15, 13130-13142.
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- 5. Nina Drašinac Pajić, Petar Djinović, Goran Dražić, Jože Grdadolnik, Primož Šket, Janez Cerkovnik, Albin Pintar, "Structural stabilization and characterization of active peroxo species on TiO<sub>2</sub> – nanotube based materials in mild catalytic wet peroxide oxidation process", *Applied catalysis. A, General*, 2018, **562**, 276-283.
- 6. Aleksander Matavž, Janez Kovač, Miha Čekada, Barbara Malič, Vid Bobnar, "Enhanced electrical response in ferroelectric thin film capacitors with inkjet-printed LaNiO<sub>3</sub> electrodes", *Applied physics letters*, 2018, **113**, 1, 012904.
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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, engineering and functional ceramics, biomaterials 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**

We employed a "Spark Plasma Sintering" (SPS) approach to prepare a dense, nanostructured, multicomponent magnet containing a high-coercivity region. For this purpose, a nanostructured powder free of heavy rare earth (HRE) was used in combination with a Dy-containing powder. We showed that this type of magnet could be manufactured in a single step by stacking both powders in the desired manner, while avoiding mixing. The short Head (since 1.4.2018): manufacturing time and the low consolidation temperature of the SPS process inhibit the diffusion of the Dy into Prof. Sašo Šturm the Dy-free region of the magnet. SEM and EDX analyses of the interface between both parts of the multicomponent specimen revealed that the microstructural characteristics and chemical compositions of the respective parts were comparable with single-component magnets prepared from the individual powders, which corresponded with the results of the magnetic characterization. In summary, magnets with locally different magnetic properties were prepared from nanostructured melt-spun ribbons using the SPS approach. The work continues with a focus on the processing of anisotropic Nd-Fe-B magnets from jet-milled powders by SPS.

As part of the research work for Slovenian industrial partners we focused on: (i) improving the coercivity of melt-spun powders used for bonded magnets, and (ii) developing a coating procedure and different coating materials to prevent corrosion in aggressive conditions. Already during the first year of the two projects we successfully increased the coercivity by more than 15% and we established the most effective solution so far to protect sensitive Nd-Fe-B powders by using alumina as a thin protective layer. We also used an electroless coating and electrochemical method for coating the basic melt spun powders with a thin Ni layer. The continuation of the work will be in (i) transferring the technology for the coercivity improvement to larger quantities of basic powder, and (ii) to perform a long-term corrosion test on the protected Nd-Fe-B powders in factory conditions. At the laboratory level, **Prof. Spomenka Kobe** we will continue the experimental work by using organic solvents in the electrodeposition of Ni. The following set of research works for the industrial partner relates to the development of a new magnetic material, which will enhance the performance of a magnetic encoder measuring system. In the framework of this project, different magnetic powders will be fabricated and characterized for their magnetic performance.

In 2018, we started with the new European project MaXycle, a transnational collaborative research and innovation project, funded from the ERA-NET Cofund on Raw Materials (ERA-MIN 2) instrument under Horizon 2020. MaXycle is developing and validating a systematic approach to overcome the barriers currently hindering a successful circular economy for Nd-Fe-B-type magnets on an industrial scale. It will provide the tools to identify different quality grades of Nd-Fe-B end-of-life magnets and provide the most suitable methods to upgrade their properties with respect to costs and sustainability for large-scale reprocessing. The project

For the industrial partner ABB (Switzerland) we developed a technology for producing Nd-Fe-B magnets with locally different magnetic properties (multicomponent magnet) that can be used in applications where only certain parts of the magnet experience strong demagnetizing fields and a significant increase in temperature.

will create a new circular economy around the sustainable supply and (re)use of precious raw materials, with the aim to recycle 15% of all the magnets produced by 2025 and will create eco-innovations, boosting competitiveness and job creation in the EU.

In the frame of the Marie Skłodowska-Curie European Training Network (DEMETER) we are focusing on the recycling of critical raw materials. We successfully produced novel permanent magnets based on recycled end-of-life Nd-Fe-B and Sm-Co systems. With the implementation of the SPS technique, we produced Nd-Fe-B permanent magnets from recycled powders obtained after HDDR (hydrogenation-disproportionation-decrepitation-recombination) processing. A 30% increase in the initial coercivity ( $H_{ci} = 1190 \text{ kA/m}$ ), with a remanent magnetization  $B_r = 0.82 \text{ T}$ , and BH<sub>max</sub> = 118 kJ/m<sup>3</sup> were achieved (published in the Journal of Alloys and Compounds). Additionally, the recycling





Head (until 31. 3. 2018):

scheme of the HDDR route has been established by relating the magnetic properties' variations with the particle size and oxygen content to help industry retain control of the microstructure and quality in recycled Nd-Fe-B powders. Moreover, the SPS method was also successfully used in the compacting of recycled HD (hydrogen-decrepitation) powders based on  $SmCo_5$ , where we achieved a RT coercivity > 2200 kA/m and at 180 °C an H<sub>ci</sub> > 1200 kA/m, an improvement over the initial powder properties due to particle size refinement during the HD recycling (reported in a publication in IEEE Transaction on Magnetics). In the frame of the DEMETER project, chemical recycling, i.e., processing of the rare earth, has been investigated. The electrodeposition of the Nd and Fe elements from ionic liquids based on 1-ethyl-3-methylimidazole dicyamide was evaluated. We found that Nd can only be reduced in the presence of Fe, which most probably catalyses the further reduction of Nd, and we also proposed an appropriate mechanism.

FRAME - A novel recycling concept for Nd-Fe-B sintered magnets was developed based on anodic etching (Patent application, European Patent Office, Application EP 18 2018 508.4). By using an organic solvent, the Nd<sub>2</sub>Fe<sub>14</sub>B matrix phase was recovered by preferential anodizing/etching of the grain-boundary phase (Nd-rich phase). Around 70 % of the magnet was recovered directly in the form of Nd<sub>2</sub>Fe<sub>14</sub>B grains, which are suitable for new magnet production. The collected rare-earth oxides and rare-earth-rich leaching solutions can be further treated and used for the production of rare-earth-based products.

In 2018, we started a national project (L2-9213) in collaboration with the company Magneti Ljubljana, d.d. where we are investigating novel ways of recycling magnetic swarfs based on Sm-Co. Novel strategies concerning

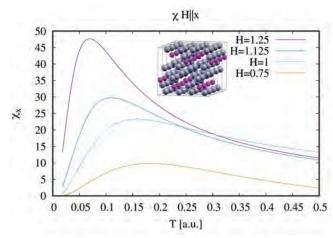


Figure 1: The calculated temperature-dependent magnetic susceptibility for a monatomic nanowire with the help of method the renormalization group of matrix density matrices (TDMRG). The  $Ce_3Al$  crystal structure with chains of Ce atoms (magenta balls) as the source of the quasi onedimensional magnetism is shown in the inset.

a)  $t_{GB} = 3 \text{ nm}$ , ferromagnetic GB b)  $t_{GB} = 6 \text{ nm}$ , non-ferromagnetic GB

Figure 2: Magnetization reversal in the case of (a) magnet with a ferromagnetic grain-boundary phase and (b) magnet with a non-ferromagnetic grain-boundary phase.

metallurgical and electrochemical recycling procedures to achieve a circular economy are currently under investigation. We found that by using an organic solvent, a  $\text{Sm}_2\text{Fe}_{17}$  sintered magnet can be selectively etched for further Sm and Co extraction.

We continued with research in the framework of the European project **AMPHIBIAN** ("AnisoMetric Permanent HybrId magnets Based on Inexpensive And Non-critical materials"). The goal of the project is to prepare hybrid ferrite-based magnets with an energy product,  $BH_{max}$ , higher than 50 kJ/m<sup>3</sup>. The upper limit so far is 45 kJ/m<sup>3</sup>. The hybrid anisotropic magnets with enhanced magnetic performance prepared in the AMPHIBIAN project will be installed in a flywheel (electric energy storage device). Such an achievement would open up an entirely new field of possible applications. Up till now we systematically studied the influence of various processing methods on the magnetic properties of Sr-hexaferrite and determined the most suitable densification method. In the past year we were also investigating possibilities for an increase in the recycling rate of the scrap material produced during the injection moulding of ferrite magnets.

On the basis of the density-functional theory we investigated the evolution of magnetic Ba-hexaferrite-based nanostructures by predicting the most probable termination planes. In a collaboration with the Department for Solid State Physics we contributed a theoretical description of the quantum-critical point in the magnetically quasi-one-dimensional system Ce<sub>3</sub>Al (Figure 1). We applied the transfer-matrix density-matrix-renormalization group (TDMRG) method in order to calculate the temperature-dependent magnetic susceptibility as a function of the external magnetic field H, which gave us the critical point. In addition, we collaborated with the Department for Solid State Physics in the investigation of the Verwey-type charge-ordering transition in a p-shell material, which does not exhibit a complex interplay between various degrees of freedom. The results were published in Science Advances (IF = 11.5).

In the frame of the ARRS postdoc project Z2-7215, we have successfully finalized the study of heavy-rare-earth fluorides' influence on the coercivity of Nd-Fe-B melt-spun ribbons. The excellent results were a starting point for a collaboration with the company Kolektor Group. In this project our mission is to establish a process that would lead to an improvement of the coercivity by 15 %, with the costs not allowed to increase by more than 10 %. With Japanese colleagues at NIMS we performed research in which we correlate the domain movement during magnetization reversal with the microstructural analyses (Figure 2). In two different types of hot-deformed

magnets the regions with misaligned grains were compared and their role in magnetization reversal was considered and consequently the coercivity difference was explained.

### **Complex Intermetallic Alloys**

In the frame of the **International Associated Laboratory (LIA) PACS2**, which connects CNRS and JSI, we are studying the crystal structure and chemistry of so-called push-pull complex metallic alloys in relation to their processing routes, final physical properties and potential applications.

We continued our studies of the crystallization mechanisms of a glass prepared by melt-spinning in the Al-RE-Fe-Cu alloys system. Gd, with a much stronger magnetic moment, followed the previous studies when using Ce. The structure of Gd-based alloys manifests a more reduced vitrification ability than that of the Ce-based counterparts, which is consistent with a 300 K higher liquidus line in the Al-Gd diagram. TEM observations of the microstructure at the atomic scale show crystallites within the glassy matrix. The temperatures Tg and Tx are higher compared to a Ce-based system, which coincides with the higher melting point of Gd. The magnetic behaviour of Gd-based glasses at RT changes from paramagnetic (PM) to ferromagnetic (FM) and the magnetization increases from 4 to 16 emu/g. Below the blocking temperature, the PM is replaced by an antiferromagnetic (AFM) state. The evidence of spin-glass behaviour appears as well. The local atomic structure of the glasses imparts a hybridization effect, which couples the adjacent magnetic moments of the constitutive elements. The ribbons of Ce- and Gd-based metallic glasses were successfully consolidated into cylinders in the range between Tg (T of glass transformation) and Tx (T of crystallization), via the SPS technique, while maintaining a glassy structure.

#### Structural Materials

In the framework of the **EUROfusion** programme, we carried out research devoted to materials for the divertor of the future Demonstration Power Station (DEMO). Namely, the divertor is expected to be exposed to a very severe environment. Currently, no material meets the requirements for use in the DEMO reactor under the proposed operating conditions. Therefore, in the High-Heat-Flux-Materials working group we are working on improving the properties of metallic tungsten, which is, unfortunately, brittle at moderate temperatures, and above approximately 1000 °C its strength is greatly reduced due to recrystallization and the excessive growth of grains. At the Department of Nanostructured Materials we have developed a new W-W<sub>2</sub>C composite, which is prepared by adding WC nanoparticles to tungsten powder and by densification using the SPS technique. We examined the material in detail and, with the help of partners in Spain, Romania and Germany, analyzed its properties across a wide range of temperatures up to 1000 °C. Improved properties in comparison to other composites have been confirmed.

In the **Enabling Research project**, we also verified the suitability of low-activation WC-based cemented carbides as a fusion-relevant material. In cooperation with the Institute for Materials and Technology (IMT) we investigated high-entropy alloys and iron triads as a binder phase in the WC-cemented carbide. The samples of WC-Ni are being tested. Both projects were also financially supported by the ARRS.

#### Sensors

We are developing modified printed electrodes via nanostructuring of the receptor elements based on transitionmetal oxides that serve as the base for an autonomic sensor platform suitable for in-situ HCHO analytical studies. We have fabricated modified Ni nanowires for the electro-oxidation of formaldehyde (HCHO), which are promising for use as an effective electrochemical receptor element. An active material (electro-catalyst) for HCHO detection was generated by the template-assisted electrodeposition of Ni into Al<sub>2</sub>O<sub>3</sub> membranes, followed by modification in

an alkaline solution (KOH), which produced an active amorphous Ni(OH)<sub>2</sub> layer on the surface. The proposed electrode shows two wide ranges of linear response and a low detection limit (0.8 µmol L<sup>-1</sup>). Furthermore, it exhibits a fast response time, a high sensitivity, good reproducibility and selectivity to other similar organic compounds. Furthermore, the Ni nanowires were successfully integrated on paper-based, screen-printed electrodes (SPE) that results in the development of new, low-cost devices for the in-situ analysis of HCHO. Acrylamide is a widely used industrial organic

With nanostructuring we are developing sensoric receptor elements with enhanced sensitivity for detecting toxic organic compounds, like formaldehyde (HCHO) (national project L2-8182) and acylamide (AA).

compound. In nature, it can be found as a contaminant originating from polyacrylamide – a polymer that is used in wastewater treatment, the paper and textile industries, and as a monomer in cigarette smoke and in heat-treated food. Due to its neuro and genotoxicity and classification as a potential human carcinogen, it is essential that we are able to detect its presence, especially in food products. We are developing modified screen-printed electrodes via nanostructuring of the receptor elements based on conducting polymers for creating molecular imprinting suitable for acrylamide analytical studies. So far, we have successfully electropolymerized polyaniline onto different gold-based SPE electrodes by using an electrochemical approach. It was prepared in a conductive emelardine form, which enables further usage in studies for designing molecularly imprinted sensing systems. With the addition of propanamide as a template molecule into the polymerization suspension, polyaniline polymerized around the template, causing its imprint confirmed with FTIR. The obtained systems, after the template molecule removal, present the first stage in the assembly of the acrylamide-sensitive receptor element.

#### Materials for Health and a Clean Environment

The results also showed the high selectivity of the FePt/SiO<sub>2</sub>/Au hybrid nanoparticles between the normal and cancerous cell line. Furthermore, the improvement in the contrast and the easier distinction between the healthy and the cancerous tissues were clearly demonstrated with *in vitro* MRI experiments, proving that hybrid NPs have

We have prepared an innovative theranostatic material based on FePt/SiO<sub>2</sub>/Au hybrid nanoparticles. *In vitro* experiments on normal and cancerous urothelial cells have proven their efficiency for both photo-thermal therapy and magnetic resonance imaging (MRI).

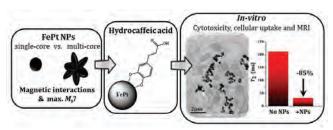


Figure 3: A study of the magnetic interactions revealed the optimal size and morphology of Fe-Pt nanoparticles with the highest saturation magnetization  $(M_s)$ . A novel biocompatible hydrocaffeic acid coating was used to prepare a highly efficient and safe MRI contrast agent, which was proven by an in vitro study.

an excellent potential to be used as a contrast agent. The research was published in the scientific journal **Nanoscale** and according to the Slovenian Research Agency's projects "**Excellent in Science**" it was ranked among the best scientific achievements of 2018.

In order to develop the **most effective contrast agent for MRI based on superparamagnetic nanoparticles**, we have investigated the effect of the magnetic interactions acting between the nanoparticles on their magnetic properties, which are crucial for their efficiency. Furthermore, a novel and biocompatible coating on hydrocaffeic acid was used for the first time. *In vitro* testing showed the non-toxicity of as-prepared nanoparticles even at high concentrations and for a longer period of time (1 week). Cellular uptake and the internalization mechanism were studied using ICP-MS and TEM analyses. Moreover, *in vitro* MRI measurements have shown that the exposure of the cells to the lowest used concentration of the HCA-Fe-Pt nanoparticles is already enough to decrease the  $T_2$  signal by 70%. This proves that HCA-Fe-Pt nanoparticles have great potential to be used as safe and very efficient MRI contrast agents. The findings of the study were published in **RSC Advances** (Figure 3).

Within the framework of the **Isofood** project, we organized a workshop on nanoparticles in food. We demonstrated the various aspects of nanoparticles entering food, either during production, packaging and cooking, or are added to improve taste, colour and consistency. They are difficult to detect in food, because they are very small, so they need specific methods

and techniques for their detection and characterization, as well as for analyzing their interactions with cells and the effects on health. In cooperation with the Faculty of Electrical Engineering, the physico-chemical properties of silver and  $TiO_2$  nanoparticles were analysed within the project "Analysis of potential harmful effects of nanoparticles and accompanying mechanisms, from physicochemical and *in vitro* characterization to the activation of the

Figure 4: Morphology factor,  $f_m$ : A new criterion for the evaluation of nanoparticle branching, allowing a comparison of morphologies regardless of the particle size. It is defined as the ratio of the particle's total surface area vs. the volume of an equivalent sphere that would correspond to the particle's volume.

innate immune system". The main aim of the research is to understand the response of the cells to the investigated nanomaterials.

We continued the study of three-dimensional silk fibroin scaffolds for their potential use in tissue engineering, regenerative medicine and pharmacy. In the framework of the project "Role of estrogens and active brain feminisation, and the development of a new hormone implant, mimicking estrous cycle", we focused on the preparation and tailoring of the fibroin scaffolds' degradability and on the controlled release of the estrogen. The results are very promising.

In the field of the **anodic oxidation** of titanium, the influence of the anodization electrolyte aging and the titanium surface treatment on the photocatalytic properties of the synthesized  $\text{TiO}_2$  nanotube films were studied. In these studies caffeine was used as a model organic molecule. In a different study,  $\text{TiO}_2$  nanotubes were used as a catalyst for the synthesis of adipic acid from 1,6-hexanediol, which is a very important scientific field still in its development phase. In cooperation with the National Institute of Chemistry, the first immobilized TiON nanotube films were prepared and used for the electrocatalytic degradation of phenol and as a catalyst support for the oxygen-evolution reaction. In the latter case, a high conductivity and specific surface area of the TiON nanotubes served as an efficient and stable substrate for an iridium catalyst. Apart from titanium,

many other metals, such as iron, nickel, vanadium, tungsten, zinc and copper, were successfully anodized and their morphologies thoroughly studied. Finally, we continued with the development of innovative reactors for the photoelectrocatalytic purification of water and the photocatalytic purification of air. The active photocatalyst in all the reactors was based on TiO, nanotubes.

Our fundamental studies of self-assembly were directed towards studies of how to exploit twinning to achieve the angular branching of rutile  $TiO_2$  mesostructures. We have shown that twin-based oriented attachment (OA) can be realized in a solvothermal process from Ti(IV)-butoxide under mild acidic conditions that favour the precipitation of rutile with a short-prismatic morphology. The aspect ratio of the precipitated nanocrystals decreases linearly with the acidity of the medium, i.e., the lower it is, the higher is the affinity for twin OA. Through the control of lateral {110} and twin {101} OA in rutile we are able to generate diverse fractal-like multiply twinned inorganic mesostructures for nanotechnology applications. To quantify the branching, we defined a morphology factor,  $f_m$ , a new generally applicable criterion, which provides a first quantitative measure of the nanoparticle morphology, and can be used to evaluate and compare the relative increase of a specific surface area for any branched materials (Figure 4). The study was published in **Crystal Growth & Design**. The aim of these studies is to explain the mechanism of self-assembly that will allow the production of hierarchic branched multifunctional mesostructures for advanced nanotechnology applications.

#### **Engineering Ceramics**

In collaboration with Madrid's CSIC (Instituto de Ciencia de Materiales de Madrid), we have developed **cellulose**, **nanofiber-reinforced**, **engineering electro-conductive ceramics** and filed a Great Britain patent application. Imparting the electrical conductivity to a dielectric ceramic with conducting nano-carbons (nanotubes or graphene) is challenging. The invention relates to an alternative, sustainable way with a small addition of cellulose nanofibers, which render highly homogeneous ceramic dispersions due to the increased hydrophilicity character and facilitates green machining of the consolidated green bodies. During sintering, the nanofibers are in-situ transformed to a 3D, percolative, few-layered-graphene network within a dense and refined ceramic matrix inducing a high electrical conductivity (Figure 5). The work was published in Nanoscale.

In collaboration with the distinguished Israeli Ben-Gurion University and Max Planck Institute, we have characterized the pore evolution and thermal properties of newly developed foam-based materials (C-N-P) targeted for fire-retardant applications. The work was accepted for publication in the renowned journal of **Angewandte Chemie International Edition**.

In the field of dental ceramics, we have traditionally been involved in the research on zirconia (3Y-TZP) as well as other dental materials conducted in collaboration with the Department for Prosthetic Dentistry, Medical Faculty, University of Ljubljana. In 2018 a basic research ARRS project was obtained entitled "Towards reliable implementation of monolithic zirconia dental restorations." In Journal of Prosthodontic Research, we have published a study on the influence of thermo-mechanical cycling on porcelain bonding to Co-Cr and Ti alloys fabricated by casting, milling, and selective laser melting. The investigation of the fracture resistance of endodontically treated maxillary incisors restored with zirconia posts, where we have studied the effect of the internal plateau preparation, was published in Advances in Applied Ceramics. Juliane Moritz from the Technical University of Dresden conducted experimental work for her diploma thesis, where she modified the surface topography of zirconia ceramics for the improved biocompatibility of dental implant surfaces. The work was recognised by Deutsche Keramische Gesellschaft and awarded Juliane with prestigious Hans-Walter Hennicke lecture prize for the best lecture given by young ceramists during the annual 2018 DKG conference that was held in Munich in April. In collaboration with Ustna Medicina d.o.o. we have developed a next-generation bioactive sealer for the endodontic treatment

The extensive, long-term research work on the exploitation of the naturally self-driven AIN powder hydrolysis that can be used as a powerful tool in advanced materials engineering was\_summarised in a personalised review article (Personal Accounts) published in *The Chemical Record*.

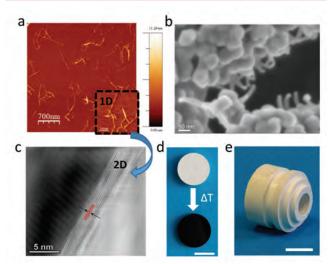


Figure 5: (a) Atomic force microscopy (AFM) micrograph of individual cellulose nanofibres (CNF) deposited on a mica substrate. The magnified inset image underlines the 1D morphology of the CNF, which is transformed into a 2D carbon phase during SPS sintering, as observable in d. (b) SEM micrograph of freeze-dried 2%CNF-zirconia powder. (c) Photograph of a machined 2% CNF-zirconia green body. (d) BF STEM image of a few-layered graphene (FLG) film between alumina grains in 3%CNF-alumina. (e) Photograph of 3%CNF-alumina before and after SPS sintering, showing a white-to-black colour change. Copyright (2018) The Royal Society of Chemistry.

A spin-out company, Genuine Technologies d.o.o., was founded that will use the JSI's licensed knowledge and provide more successful treatments for patients.

of teeth with improved bioactive, rheological (handling) and chemical properties, described in a technical innovation.

#### Functional Ceramics

In the field of **oxide thermoelectric materials** of the n-type, we proceeded with the development of **ZnO ceramics**. In cooperation with Laboratoire CRISMAT from Caen (France) we studied the structural characteristics and thermoelectric properties of ZnO ceramics doped with extremely low quantities of In. ZnO(In) ceramics were synthesized using a simple solid-state process. The structural features and thermoelectric properties of the  $Zn_{1-x}In_xO$  series with an ultra-low indium content ( $0.00 \le x \le 0.02$ ) were assessed. HAADF-STEM analyses indicate that indium has the ability to create multiple basal plane (*b*-IB) and pyramidal (*p*-IB) defects that produce domains with inverted polarity, starting from dopant concentrations as low as 0.25 atom % (Figure 6). Interestingly, the formation of IBs causes increased phonon scattering, while increasing the electrical conductivity, and thereby

This study is a step forward to the design of other thermoelectric materials where dopantinduced planar defects in bulk transition-metal compounds have the potential to enhance both phonon scattering and electronic conductivity.

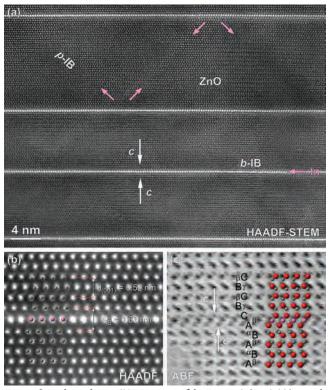


Figure 6: High-resolution STEM images of the Zn  $_{1}$  Nn  $_{2}$ O (x = 0.02) sample viewed along the [100]ZnO zone axis. (a) HAADF-STEM overview with parallel b-IBs composed of strong white dots, corresponding to In-atomic column positions, interconnected by dark diffuse p-IB defects (marked by pink arrows at about 45°). (b) HAADF-STEM image close-up of b-IB section with overlaid cationic column positions and (c) corresponding ABF-STEM image with O-columns that allow determining the atom layer stacking and polarity (inverted c-axis) (red, 0; gray, Zn; pink, In). From an article published in ACS Appl. Mater. Interfaces, 10, (2018), 6415-6423.

enhancing the overall thermoelectric properties. This is a completely new finding for ZnO ceramics with such low additions of In, showing that we do not have classic solid solubility of In in ZnO, but the inverse boundaries (IBs) are immediately formed. The study is a result of a continued collaboration with the French group and was published in ACS applied materials & interfaces (IF=8.456).

According to recent findings that magnetic semiconductors have better thermoelectric properties than expected, we began to study the effects of magnetic dopants on the thermoelectric properties of ZnO ceramics. The first analysis of the samples with the composition  $Zn_{0.98x}Al_{0.02}Co_xO$  (x = 0, 0.001, 0.0025, 0.005, 0.01, 0.05, 0.10) showed that the ceramics sintered at 1400°C became paramagnetic when doped with Co. Further research will focus on studying the possible effects of Co and magnetism on the density and mobility of charge carriers, the Seebeck coefficient and the electrical conductivity.

In the field of varistor ceramics, in cooperation with the "Shanghai Institute of Ceramics, the Chinese Academy of Science - SICCAS" we continued with the research and development of a new type of varistor ceramics that do not contain standard dopants for current-voltage (IU) nonlinearity, such as oxides of Bi, Ba, V and Pr. They are distinguished by high I-U nonlinearity and a very low addition of dopant, none of them melting or having high vapour pressure at the sintering temperature, which means great advantages in comparison with the classic varistor ceramics and multilayer chip varistors, our investigations about the influence of the composition and the sintering regime on the microstructure development and I-U characteristics of ZnO-Bi<sub>2</sub>O<sub>3</sub> varistor ceramics at temperatures below 1000 °C are important. We have developed varistor ceramics that have excellent I-U characteristics for applications after sintering at temperatures between 800 and 950°C. The results are reported in the journal **Ceramics-Silikaty**.

We investigated the effects of the dual doping of  $\text{SnO}_2$  varistor ceramics with CoO and Nb<sub>2</sub>O<sub>5</sub> on the formation of twin boundaries, microstructure development and electrical properties by electron microscopy methods. With the addition of Nb<sub>2</sub>O<sub>5</sub>, densification is shifted to higher temperatures (1430°C), producing a coarse-grained microstructure composed of twinned SnO<sub>2</sub> grains. Already a small addition of Nb<sub>2</sub>O<sub>5</sub> (0.1 mol%) triggers a three-fold increase in growth rate via the diffusion-induced grain-boundary mobility (DIGM) due to the formation of oxygen vacancies in the grain-boundary region. At 0.5 mol% of Nb<sub>2</sub>O<sub>5</sub> chemical equilibrium is achieved and the SnO<sub>2</sub> grains undergo normal grain growth. Electron back-scatter diffraction (EBSD) has shown that the prevailing type of twins

is {101}. Cyclic twins are common. HAADF-STEM analysis revealed a nonuniform segregation of Nb along the twin boundaries, indicating that they are not directly triggered by the addition of the dopant, but are most probably a result of a yet unexplained sequence of topotaxial replacement reactions. Using energy-dispersive spectroscopy (EDS) we have shown that by the dual doping of SnO<sub>2</sub> with CoO and Nb<sub>2</sub>O<sub>5</sub> the amount of Co dissolved in the SnO<sub>2</sub> grains is ~4× lower compared to the amount of Nb. We proposed the following charge-compensation mechanism: 6 Sn(IV)Sn × (IV)  $\Rightarrow$  Sn(II)Sn "(IV) + Co(II)Sn "(IV) + 4 Nb(V) · Sn(IV) where oxygen vacancies, generated by the acceptor dopants Sn<sup>2+</sup> and Co<sup>2+</sup>, are compensated by one vacancy on the tin lattice site. The optimal electrical properties were achieved for the  $SnO_2-1$  mol% CoO-1 mol%  $Nb_2O_5$  sample displaying the highest nonlinear coefficient ( $\alpha$ =50), matching those of ZnO-based varistors, while higher additions of  $Nb_2O_5$  (>1.0 mol%) result in a collapse of the nonlinearity and a sudden increase in the leakage current. The study was published in **Ceramics International**.

#### Minerals

In collaboration with the Department for Litospheric Research of Vienna University we contributed to their study of spinel (MgAl<sub>2</sub>O<sub>4</sub>) formation during a replacement reaction between corundum (Al<sub>2</sub>O<sub>3</sub>) and periclase (MgO), involving the reorganization of Al atoms in octahedral interstices, the incorporation of Mg atoms into tetrahedral sites and a transition from the hexagonal close-packed (*hcp*) to the cubic close-packed (*ccp*) oxygen (O) sublattice. For the first time we show this type of transformation as a progressive diffusion-controlled process at the atomic scale using quantitative HAADF-STEM. Spinel forms in a progressive zipper-like interface motion, in which MgAl<sub>2</sub>O<sub>4</sub> adopts two crystallographic orientations related by the 180° rotation in the (111)<sub>ss</sub> | | (0001)<sub>ccm</sub> interface. Intergrowth of these domains generates a new type of coherent (111) twin boundaries in spinel that have previously not been reported. This is a case study of topotaxial replacement reactions involving the *hcp/ccp* transition in general. It was published in **Acta Crystallographica A** (IF=7.93). Further research subjects are in progress, including a study of Fe- Ti micro- inclusions as carriers of rock magnetism from the Mid- Atlantic ridge (starts in March 2019) and the study of garnet inclusions.

#### Analytical Electron Microscopy

For the characterization of materials on the micro- and submicrometer scales we use the advanced analytical methods of high-resolution scanning electron microscopy (FEGSEM), qualitative and quantitative elemental analysis by electron-probe microanalysis (EPMA) using energy-dispersive and wavelength-dispersive X-ray spectroscopy (EDS, WDS), electron-backscatter diffraction (EBSD) and complementary atomic force microscopy (AFM).

With the implementation of correlative microscopy, i.e., by using an optimum combination of FEGSEM, EDS, WDS, EBSD and AFM methods and taking into account the characteristics of the individual materials, we achieved reliable, precise and accurate analytical results. We studied various materials such as ceramic thermoelectrics,

complex metallic and quasicrystalline alloys, magnetic materials based on Nd-Fe-B and Sm-Co, abrasives, piezoelectric perovskite ceramics. Among other things, we examined the influence of heat treatment on the microstructure and phase composition in Al-Cr-Sc alloys. By performing the expert-level quantitative WDS microanalysis we have accurately measured trace concentrations of the dopants Eu and Dy in phosphorescent ceramics based on Sr<sub>4</sub>Al<sub>14</sub>O<sub>25</sub>; we have determined the exact chemical composition of submicrometric ceramic thin films that were made from 67PMN33PT complex perovskite. Using micro-crystallographic EBSD analyses, we directly confirmed the presence of icosahedral and decagonal quasicrystals in complex alloys based on Al-Mn (Figure 7), we investigated and determined the type of twins in cassiterite SnO<sub>2</sub> ceramics, and we studied the texture in Nd<sub>2</sub>Fe<sub>14</sub>B magnetic materials.

The ESTEEM consortium (Enabling Science and Technology through European Electron Microscopy) continued its activities in the field of materials characterization using state-of-the-art techniques of transmission electron microscopy, such as electron energy-loss spectroscopy (EELS), high-resolution scanning transmission electron microscopy (STEM, HAADF-STEM) and the mechanical preparation of the TEM samples.

The research group of the Department for Nanostructured Materials is very strongly connected with the activities within the **Center for Electron** 

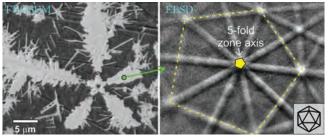


Figure 7: FEGSEM micrograph of dendritic quasicrystals in Al-Mn alloy and the corresponding EBSD pattern, which directly confirms the 5-fold symmetry of the icosahedral quasicrystal.

The ESTEEM consortium has the status of an EU Advanced Community, and a lot of effort was focused on the preparation of a new project proposal for ESTEEM3, which was successfully granted in 2019. A member of our department is the scientific coordinator of the consortium.

Microscopy and Microanalysis (CEMM), mainly through the implementation of various electron microscopy analytical techniques and the possibility for the researchers to access the research infrastructure for electron microscopy.

#### Industrial partners

We have conducted analyses of innovative composite abrasives for the industrial partner Weiler Abrasives - SwatyComet within the project "Microstructural investigations of abrasive materials", which are intended to develop and manufacture improved cutting and grinding tools with a prolonged lifetime.

#### Education and outreach activities.

For the sixth year, the members of the department participated in science-promotion activities within the framework of the Science on the Street (ZnC) project. In 2018 there were 18 popular science lectures, a scientific slam, and a round table. On the ZnC website we have published 19 blogs of researchers and 2 contests. In cooperation with the Slovenian Fusion Association, IJS, we co-organized a professional excursion to the ITER fusion reactor that is under construction.

### Awards and appointments

- 1. **Department for Nanostructured Materials**, the European project REProMag, German Prize for Efficient Use of Raw Materials 2017 (Deutscher Rohstoffeffizienz-Preis 2017, given in January 2018. Prestigious Award received by EU research project REProMag where the Department for Nanostructured Materials was one of the 14 partners from 5 countries, which successfully developed the technological process of re-use of recycled rare-earth magnets, which enables economically efficient production of magnetic parts with complex structures and geometry and 100% free of waste material along the entire production chain (http://www.repromag-project.eu/).
- Benjamin Podmiljšak, Award for the best poster at the 2nd IEEE Conference on Advances in Magnetics; AIM2018, La Thuile, Italy, 3–10 February 2018. Title of the awarded contribution: "Tailored metal injection moulding of isotropic NdFeB hard magnets based on recycled powders with and without Nd-additions".
- Matej Kocen, Award for the best poster and oral presentation at the 26th International Conference on Materials and Technology, 26 ICM&T, Portorož, Slovenia, 3–5 October 2018. Title of the awarded contribution: "Capturing the Sun in a tungsten 'box'" (co-authors: Petra Jenuš, Saša Novak Krmpotič, Andreja Šestan)
- 4. Nina Kostevšek, Candidate for "Excellent in Science 2018", given by members of the Scientific Research Council of Technology, Slovenian Research Agency (ARRS). Selected Achievement: "Hybrid nanoparticles for cancer treatment and diagnostics". Ljubljana, Slovenia, 23 October 2018.

#### Organization of conferences, congresses and meetings

- 1. The 26th International Conference on Materials and Technology 26. ICM&T, 3–5 October 2018, Portorož, Slovenia (co-organisers)
- 2. Annual meeting of LIA PACS2: International Associated Laboratory; Push-Pull Alloys and Complex Compounds: from bulk properties to surface functions, 17–20 December 2018, Ljubljana, Slovenia
- ISO-FOOD Spring School & Workshop on Nanoparticles and Food, 9–13 April 2018, Ljubljana, Slovenia (organisers)
- Kick-off meeting of Maxycle project: A novel Circular Economy for Sustainable RE-Based Magnets (ERA. MIN2), Goriška Brda, Slovenia, 6–8 May 2018
- Annual Meeting of Slovenian Fusion Association SFA, Podgorica, Slovenia, 20 December 2018 (coorganisers)
- 6. Workshop on "Opportunities of cooperation in the field of complex metallic alloys";
- 7. 2<sup>nd</sup> phase SRIP ToP, "New materials" value chains and the horizontal network "Modern Production Technology for Materials", Ljubljana, Slovenia, 19 December 2018 (organisers)
- Expert meeting on the topic of the project application under Horizon 2020; Building a water-smart economy and society ter Microorganism communities for plastics bio-degradation (RIA), Ljubljana, Slovenia, 7 December 2018

### INTERNATIONAL PROJECTS

- K7, CTT ID Creations; Rights and Obligations regarding the Development, Use and Commercialization of Hydrothermally Synthetized TiO2 Coatings in Metal Orthopaedic and Dental Implants Prof. Saša Novak Krmpotič
  - I d Creations Oy
- Spark Plasma Sintering (SPS) of Cost Effective and High Performance Rare-Earth Based Permanent Magnets for Electrical Machines Prof. Spomenka Kobe
- ABB Switzerland Ltd
- 7 FP; ERA CHAIR ISO-FOOD Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability
- Prof. Saša Novak Krmpotič European Commission
- COST MP1407 e-MINDS; Electrochemical Processing Methodologies and Corrosion Protection for Device and Systems Miniaturization

Prof. Kristina Žužek Rožman Cost Office

- COST CA17140 Nano2Clinic; Cancer Nanomedicine From the Bench to the Bedside Dr. Nina Kostevšek Cost Association Aisbl
- H2020 DEMETER; Training Network for the Design and Recycling of Rare-Earth Permanent Magnet Motors and Generators in Hybrid and Full Electric Vehicles Prof. Kristina Žužek Rožman
- European Commission 7. H2020 - STEM4youth; Promotion of STEM Education by Key Scientific Challenges and their Impact on Our Life and Career Perspectives Dr. Luka Suhadolnik
  - European Commission
- H2020 AMPHIBIAN; Antisometric Permanent Hybrid Magnets based on Inexpensive and Non-Critical Materials Dr. Petra Ienuš
  - European Commission
- 9. H2020-EUROfusion-Plasma Facing Components-1-IPH-FU, EUROFUSION

Prof. Saša Novak Krmpotič European Commission

- Huropean Commission Materials-PPPT-FU
   Prof. Saša Novak Krmpotič
   European Commission
- European Commission 11. H2020 EUROfusion - Education-ED-FU Prof. Saša Novak Krmpotič
  - European Commission
- H2020 EUROfusion ER-4-FU; Enabling Research Prof. Saša Novak Krmpotič
- European Commission 13. Synthesis of Core/Shell MgAl2O4 Spinel Powders for Transparent Armor and IR Applications – CSMASP
  - Prof. Slavko Bernik
  - Slovenian Research Agency
- 14. Crystal and Electronic Structure of NbS3 Phases Prof. Sašo Šturm
  - Slovenian Research Agency
- Crystallography, Twinning and Phase Transformations in Minerals with Aragonite-Type Structure (CaCO3, SrCO3, BaCO3, PbCO3) Prof. Aleksander Rečnik
- Slovenian Research Agency
- 16. Characterization of Structural Defects in Semiconductor ZnO Films Grown by Atomic Layer Deposition (ALD)
- Prof. Aleksander Rečnik Slovenian Research Agency
- 17. Advanced Electronic Ceramics for the Sustainable, Efficient and Safe Use of Energy Prof. Slavko Bernik
- Slovenian Research Agency 18. Hydrous Defects and Twinning in Silicates
- Asst. Prof. Nina Daneu Slovenian Research Agency
- 19. Tungsten-Based Composite for Fusion Applications Prof. Saša Novak Krmpotič
- Slovenian Research Agency 20. Atomic-Scale Investigations of Twinning and Polytypism in Natural Diamonds Prof. Aleksander Rečnik
- Slovenian Research Agency
- Properties of Monolithic and Composite Advanced Ceramics obtained by Conventional and Non-Conventional Sintering Methods Dr. Petra Jenuš

Slovenian Research Agency

- 22. Functionalized TiO2 Nanostructures for Application in Photo-Catalysis and Sensors Prof. Miran Čeh
- Slovenian Research Agency23. Stability via Doping: Experimental and Theoretical Design of Functional Oxide Ceramics
- Prof. Aleksander Rečnik
- Slovenian Research Agency
- Micro-to Nanoscale Textures of Ore Minerals: Methods of Study and Significance Dr. Janez Zavašnik Slovenian Research Agency

### RESEARCH PROGRAMS

- 1. Nanostructured Materials Prof. Spomenka Kobe
- Ceramics and complementary materials for advanced engineering and biomedical applications Asst. Prof. Andraž Kocjan

### R & D GRANTS AND CONTRACTS

1. High-Performance Nanostructured Coatings - breakthrough in concentrated solar power

Asst. Prof. Andraž Kocjan

 Evaluation of possible harmful effects of nanoparticles and underlying mechanisms – from physico-chemical and in vitro toxicity characterisation to innate immune system

### VISITORS FROM ABROAD

- Philipp Stass, Gymnasium Borbeck, Essen, Germany, 28 January 10 February 2018
   Dr. Pavel Gavryushkin, Sobolev Institute of geology and mineralogy SB RAS, Numerical Distributed Distributed in 1, 10 Peterson 2010
- Novosibirsk, Russia, 1–10 February 2018
   Dr. Lavinia Scherf, ABB Schweiz AG, Baden-Dättwil, Switzerland, 20–21 February 2018
   Der Gutter W. Or View, Schweiz Hubertein, Der der Gebruary 2018
- 4. Prof. Cleva W. Ow-Yang, Sabanci University, Faculty of Engineering & Natural Science, Istanbul, Turkey, 22 March 2018

activation Prof Saša Novak Krmpotič

- Role of estrogens in active brain feminisation? and development of a novel hormone implant, mimicking estrous cycle
- Prof. Saša Novak Krmpotič
  Characterization of fractal structures and scale-up parameters in their synthesis Dr. Mateika Podlogar
- W- and WC-based composites for high thermally loaded parts in the fusion demonstration power plant DEMO Prof. Saša Novak Krmpotič
- Catalytically-assisted high efficiency and low-cost nanostructured sensors based on modified screen printed electrodes for analytical chemistry Prof. Kristina Žužek Rožman
- Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems
- Prof. Aleksander Rečnik8. Towards reliable implementation of monolithic zirconia dental restorations Dr. Andraž Kocjan
- 9. UV sensors nanoparticles embedded into PA fibres Prof. Spomenka Kobe
- Effective recycling of abrasive sludge in the production of Sm2Co17 magnets for a waste-free economy
- Prof. Kristina Žužek Rožman
  11. Developement of multifunctional hybrid liposomes for active cancer treatment and multimodal diagnostics
- Dr. Nina Kostevšek 12. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Sašo Šturm
- Ministry of Economic Development and Technology
- 13. A novel ciruclar economy for sustainable RE-based magnets Prof. Spomenka Kobe
- Ministry of Education, Science and Sport 14. Services for the Exports
- Dr. Zoran Samardžija
- Advanced Methods and Technologies for Processing of a New Generation of ZnO-based Varistor Ceramics Prof. Slavko Bernik
- Chinese Academy of Sciences
- 16. External Services
- Asst. Prof. Andraž Kocjan

### NEW CONTRACTS

- Corrosion protection of magnetic powders to improve their resistivity to liquids at higher temperatures
   Definition of the protection of the protecti
  - Prof. Spomenka Kobe Kolektor Group d. o. o.
- Implementation of surface modification of Nd-Fe-B powders to increase the coercivity of bonded magnets
   Deef Coercivity Veha
  - Prof. Spomenka Kobe Kolektor Group d. o. o.
- The corrosion resistivity of Nd-Fe-B powders in an aggressive environment Prof. Spomenka Kobe Sieva d. o. o.
- Effective recycling of abrasive sludge in the production of Sm2Co17 magnets for a waste-free economy
- Prof. Kristina Žužek Rožman Magneti Ljubljana, d. d.
- 5. EPP enhanced powder properties Prof. Sašo Šturm
- RLS Merilna tehnika d. o. o.
- NexGenHVEC: Advanced materials, technologies and prototypes for cost effective hybrid varistor electronic components with improved thermal stability Prof. Sašo Šturm Kekon d. o. o.
- Coating of Nd-Fe-B powders for corrosion protection transfer to pilot production Prof. Spomenka Kobe
  - Sieva d. o. o.
- 5. Prof. Mehmet Ali Gülgün, FENS, Sabanci University, Istanbul, Turkey, 4 April 2018
- Dr. Martina Lorenzetti, GE Healthcare Life Sciences, Cardiff, Great Britain, 12–15 April 2018
- 7. Dr. Blaž Belec, University of Novi Gorici, Nova Gorica, Slovenia, 16 April 2018
- 8. Dr. Ismail Ozgur Ozer, Anadolu University, Eskişehir, Turkey, 17-22 April 2018



- Nicolas Cinq, Ecole des Mines Nancy- University of Lorraine, Nancy, France, 16 April 1 September 2018
- Prof. Michel Hehn, Institut Jean Lamour, University of Lorraine, Nancy, France and Dr. Jacim Jacimović, ABB Switzerland Ltd., Baden-Dättwil, Switzerland, 3–4 May 2018
- Matej Baláž, Institute of Geotechnics, Slovak Academy of Sciences, Košice, Slovakia, 5–13 May 2018
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- Asst. Prof. Gülten Sadullahoğlu, Bülent Ecevit University, Zonguldak, Turkey, 20 June 15 September 2019
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- Muhammad Awais, University of Birmingham, Birmingham, Great Britain, 15 July 8 September 2018
- Dr. Aleksandra Dapčević, Vesna Ribić, Dr. Goran Branković, Dr. Jelena Rogan, University of Belgrade, Belgrade, Serbia, 6–17 August 2018
- Prof. Takao Mori, National Institute for Materials Science (NIMS), Tsukuba, Japan, 12-14 August 2018
- 21. Cesare Ormelli, Politecnico di Torino, Torino, Italy, 1 October 2018 31 January 2019

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- 1. Prof. Slavko Bernik
- 2. Prof. Miran Čeh
- 3. Asst. Prof. Nina Daneu, 01.05.18, transferred to Department K9
- 4. Prof. Jean Marie Dubois
- 5. Prof. Spomenka Kobe, Head, until 31.03.18
- 6. Asst. Prof. Andraž Kocjan
- 7. Asst. Prof. Matej Andrej Komelj
- 8. Prof. Saša Novak Krmpotič
- 9. Dr. Matejka Podlogar
- 10. Dr. Benjamin Podmiljšak
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- 13. Prof. Sašo Šturm, Head, since 01.04.18
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- 19. Dr. Aljaž Iveković, on leave 01.03.16
- 20. Dr. Petra Jenuš
- Dr. Petra Jenus
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- 22. Dr. Marko Soderžnik
- 23. Dr. Luka Suhadolnik
- 24. Dr. Tomaž Tomše
- 25. Dr. Janez Zavašnik

- Prof. Guorong Li, Prof. Zhenyong Man and Prof. Xiangyan Kong, Chinese Academy of Science and Shanghai Jiao Tong University, Shanghai, China, 2–7 October 2018
- 23. Dr. Aleksandar Pačevski, Faculty of Mining and Geology, University of Belgrade, Belgrade, Serbia, 10–12 October 2018
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- 30. Dr. Andreja Gajović, Ruđer Bošković Institute, Zagreb, Croatia, 3-5 December 2018
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- Prof. Michael Coey, School of Physics, Trinity College Dublin, Ireland, 7 December 2018
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### Postgraduates

- 26. Bojan Ambrožič, B. Sc.
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- 28. Dijana Đeorđić, B. Sc., left 01.12.18
- 29. Hermina Hudelja, B. Sc.
- 30. Awais Ikram, B. Sc.
- 31. Vanja Jordan, B. Sc.
- 32. Luka Kelhar, B. Sc., left 26.10.18
- 33. Matej Kocen, B. Sc.
- 34. Matic Korent, B. Sc.
- 35. Monika Kušter, B. Sc.
- Ana Lazar, B. Sc.
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- 38. Muhammad Farhan Mehmood, B. Sc.
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- 40. Sara Tominc, B. Sc.
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- 46. Tomislav Pustotnik

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#### INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Eva Pellicer, Martina Lorenzetti, Jordina Fornell, Maria D. Baró, Saša Novak, Jordi Sort, "Progress Beyond the State-of-the-Art in the Field of Metallic Materials for bioimplant applications", In: Fatima Živić (ed.), Biomaterials in clinical practice: advances in clinical research and medical devices, 2018, 25-46.

#### MENTORING

- 1. Vanja Jordan, Mesocrystal self-assembly of hierarchic rutile-type TiO2 structures: doctoral dissertation, Ljubljana, 2018 (mentor Aleksander Rečnik)
- 2. Luka Suhadolnik, Titania nanostructures based photocatalytic and photoelectrocatalytic reactors: doctoral dissertation, Ljubljana, 2018 (mentor Miran Čeh).
- 3. Tomaž Tomše, Novel multicomponent Nd-Fe-B permanent magnets: doctoral dissertation, Ljubljana, 2018 (mentor Spomenka Kobe; comentor Jean-Marie Dubois).

# **DEPARTMENT FOR MATERIALS SYNTHESIS**

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.

New methods for nanoparticle synthesis are continuously being developed. In 2018 the focus was on the hydrothermal synthesis of Sc-substituted barium-hexaferrite nanoplatelets. The hexagonal nanoplatelets, only few nm thick and approximately 50 nm wide, display unique magnetic properties, defined by their very large, uniaxial magnetic anisotropy with the easy axis 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 based on a magneto-mechanical approach in medicine. The recent development of new potential applications and Head: interests from industry dictates the need for modifications of the synthesis procedures, which will facilitate the Prof. Darko Makovec scale-up up to mass production. The hints where to search for the further improvement of our synthesis method, which will enable better control of the particle size, further improvement of magnetic properties, and facilitate the



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scale up, came from our systematic study of the nanoplatelet structure with atomic-resolution scanning-transmission electron-microscope (ARM). The ARM showed poor chemical homogeneity of the nanoplatelets (see below). The introduction of intensive stirring of the reaction mixture during hydrothermal synthesis had an unexpectedly large influence on the development of the nanoplatelets' morphology. This enabled control of the nanoplatelets' size in a broader range. Even more important, the

The distinct structure of barium-hexaferrite nanoplatelets evolves in a stepwise manner in parallel with the development of their size and morphology during hydrothermal synthesis.

procedure became more robust; the influence of experimental parameters, such as the final temperature and heating rate, which are difficult to control in large autoclaves, had a much smaller influence on the final product compared to the previous procedure.

The research devoted to the adaptation of the crystal structure to the small size of nanoparticles was focused on the structure of hexaferrite nanoplatelets. Namely, the size confinement effect on the structure is especially pronounced in mixed oxides with a complex, layered crystal structure. We

used the case of hexaferrite to reveal the general mechanism of layeredstructure adaptation to a small size of nanoparticles. The hexaferrite structure can be presented in terms of two alternating structural layers: a hexagonal  $(BaFe_6O_{11})^2$  R layer and a cubic  $(Fe_6O_9)^{2+}$  spinel S layer, forming the RSR\*S\* stacking sequence. When a material with a layered structure, such as hexaferrite, is prepared in the form of nanoparticles, it adopts a specific structure and composition defined by the termination of the nanoparticle at its surfaces with a specific, low-energy atomic layer. After hydrothermal synthesis in the presence of a high concentration of hydroxyl ions the barium-hexaferrite nanoplatelets exhibit the structure defined by a termination at the Ba-containing planes, and as the result, the Ba-rich composition. However, during subsequent washing of the nanoplatelets with water the upper two atomic layers are dissolved from the basal surfaces and the nanoplatelets' structure terminates with the complete S structural block and have an Fe-rich composition. Moreover, the crystal structure of the hexaferrite nanoplatelets can only evolve in a

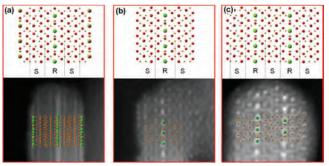


Figure 1: Structural models and atomic-resolution HAADF STEM images illustrate the development of the Ba-hexaferrite nanoplatelet structure during hydrothermal synthesis: (a) initial nanoplatelet, (b) nanoplatelet after washing with water, (c) nanoplatelet after exaggerated growth.

stepwise manner in parallel with the development of their size and morphology. During hydrothermal synthesis the primary, ultrafine hexaferrite nanoplatelets form by reactions between Ba- and Fe-hydroxides at temperatures below 80 °C. They display a structure that can be represented by a SRS\* segment of the RSR\*S\* unit cell. Due to the stable SRS\* structure, the thickness of the primary nanoplatelets remains unchanged up to approximately 150 °C, when some of the primary nanoplatelets start to grow exaggeratedly and their thicknesses increase discretely

with the addition of the RS segments to their structure (Figure 1). The SRS\* structure of the primary nanoplatelets is too thin for the complete development of the magnetic ordering. However, the addition of just one RS segment (i.e., SRS\*R\*S structure) gives the nanoplatelets hard magnetic properties, with a modest saturation magnetization,  $M_{s}$ , ~15 emu/g.

A breakthrough in applications of the BHF nanoplatelets was enabled by our discovery that their  $M_s$  can be increased to over 30 emu/g already during the hydrothermal synthesis with addition of Sc. The increase was not expected since the Sc substitution is known to greatly decrease the magnetization of the bulk hexaferrite. Moreover, the  $M_s$  of the Sc-substituted hexaferrite nanoplatelets showed unexpected decrease with their size. In 2018 we completed the study devoted to this extraordinary finite-size effect, which showed for the first time that a chemical substitution can have an opposite effect on the magnetic properties of nanoparticles compared to the bulk. A combination of atomic-resolution imaging and elemental mappings with ARM showed that the Sc<sup>3+</sup> ions substitute the Fe<sup>3+</sup>

The extraordinary finite-size effect of the Sc substitution on the magnetic properties of barium-hexaferrite nanoplatelets was analysed. ions preferentially in the R block of the hexaferrite SRS\*R\* structure in the nanoplatelets, similar to the bulk. Unexpectedly, the Sc was inhomogeneous distributed over the nanoplatelets' structure; in the nanoplatelet, which only contained two R blocks, i.e., SRS\*R\*S structure, the Sc was frequently concentrated in only one of the R blocks. This inhomogeneous distribution

of Sc across the individual nanoplatelets made a strong indication, where to search for the improvements in the synthesis procedures. On the other hand, it revealed some structural details that would probably remain hidden if the Sc was to be homogeneously distributed. A clear difference between the nano and the bulk was detected with quantitative analysis of the HAADF images performed in cooperation with Prof. Goran Dražić from the National Institute of Chemistry (Slovenia). For the first time we showed that in the nanoplatelets the Sc<sup>3+</sup> ions can partially substitute the Ba<sup>2+</sup> ions and not only Fe<sup>3+</sup> ions, as reported for the bulk. The substitution of Ba<sup>2+</sup> ions for smaller Sc<sup>3+</sup> ions resulted in an unexpected, large local expansion of the structure, which was explained by the presence of Ba vacancies formed for the compensation of the extra charge. However, the Sc<sup>3+</sup> substitution for the Ba<sup>2+</sup> cannot explain the large increase in the  $M_{s'}$ . Ab-initio calculations performed in cooperation with Prof Matej Komelj from the Department for Nanostructured Materials, JSI, suggested that the opposite effect can be ascribed to specific, two-dimensional magnetic ordering in the thin nanoplatelets.

For applications of the nanoparticles, as well as for their assembly into composite materials, engineering of their surface properties is of key importance. The surface properties are usually engineered by bonding different functionalization molecules onto the nanoparticles' 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. Since irreversible covalent bonding is not possible between inorganic surfaces and organics, an alternative coordinative bonding is

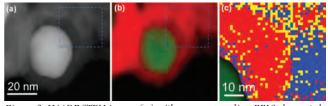


Figure 2: HAADF STEM image (a) with a corresponding EELS elemental map (Fe-green, C-red) (b). Figure (c) shows a map of the expanded area marked with a rectangle on Figures (a) and (b), which shows the distribution of graphitic carbon (red) and non-graphitic carbon (blue).

often exploited for the surface functionalisation. Very strong coordinative bonding can be achieved between surface metal ions and some organic moieties (e.g., carboxylates, sulfonates, phosphonates). Among those, the phosphonates are known to form the strongest coordinative bonds, especially with trivalent metals like Fe<sup>3+</sup> and lanthanides. This strong interaction is possible due to three electron-donating O atoms from the phosphonic group ( $\text{RPO}_3\text{H}_2$ ,  $\text{ROPO}_3\text{H}_2^-$ , or  $\text{RPO}_3^{-2-}$ ). Consequently, the phosphonic group can bridge (i.e., chelate) two metal ions, forming a very stable chelating bond. In addition, metal phosphonates are thermally stable and poorly soluble in water, making them a possible alternative to silica coatings. Our first study was focused on a specific tetraphosphonate, ethylenediamine tetra(methylene phosphonic acid), shortly EDTMP, for coating the surfaces

of barium hexaferrite nanoplatelets. Few-nanometre-thick amorphous coatings formed under various synthesis conditions (ligand concentration, temperature, pH, time). Surprisingly, the coatings were thicker than calculated from the possible surface coverage, determined with a thermogravimetric analysis. A more detailed ARM study revealed the depletion of the nanoplatelets' surface Fe<sup>3+</sup> ions and their incorporation into an amorphous coating. This suggest that a metal-phosphonate framework was formed on the nanoplatelets surface. Moreover, the unexpectedly large coating thickness also suggests its high porosity. The new hybrid materials composed of a magnetic core hybridized with a porous framework with many active sites (npr., -OH, P=O, P–O, =NH<sup>+</sup>) are candidates for new recyclable magnetic catalysts or chemical reactors. The study continues in cooperation with the Department for Complex Matter (Dr. Alenka Mertelj and Patricija Hribar Boštjanjčič), the Department of Surface Engineering and Optoelectronics (Dr. Janez Kovač) and the University of Nova Gorica (Prof. Matjaž Valant and Dr. Andraž Mavrič).

An important part of the research at the department remains devoted to clusters of superparamagnetic iron-oxide nanoparticles (nanoclusters). The nanoclusters are developed for applications that require manipulation with an applied magnetic field. The applications range from magnetic drug delivery to magnetic separation of poisonous

heavy metals from water or (bio)catalysts from a reaction mixture after a completion of a catalytic process. For the use in industrial-scale processes magnetic nanoclusters have to be produced using simple, inexpensive, and scalable methods.

A precursor material for the preparation of carbon-coated magnetic nanoclusters was synthesized by the hydrothermal carbonization of carbohydrate in the colloidal suspension of superparamagnetic iron-oxide nanoparticles. The carbon layer was formed by pyrolysis of the carbonaceous precursor. The temperature and time of pyrolysis have a major impact on the composition and the surface properties of the carbon-coated magnetic nanoclusters,

such as the amount of oxygen surface groups, the content and size of graphite nanocrystals, the specific surface area, and the pore volume and size distribution. The Raman spectroscopy and X-ray powder diffraction suggested that the Fe or Fe<sub>3</sub>C phases that formed with a reduction of iron-oxide nanoparticles during the pyrolysis catalyse the formation of

# Development of nanoclusters with highly porous silica shell for targeted drug delivery.

nano-graphite. The combination of ARM imaging and electron-energy-loss spectroscopy (EELS) (Figure 2) clearly showed that nano-graphite shells formed exclusively around the Fe<sub>3</sub>C phase, explaining their remarkable stability against oxidation. The study shed light on a mechanistic aspect of the transition-metals-catalysed-graphitization of carbohydrate-derived precursor. For applications based on heating with excitation in an alternating magnetic field, the material has to retain soft-magnetic properties with high susceptibility. As the Fe<sub>3</sub>C decreases the susceptibility of material we developed a new synthesis procedure, which delays its formation. Consolidation of the precursor in a pre-annealing step retained the magnetic phase in the form of soft-magnetic iron oxide. The developed nanoclusters demonstrated the superior heating capability in an AC magnetic field.

N-doped carbonaceous/graphitic materials are gaining a lot of interest in catalysis because of their unique electronic properties. In such materials N can be present as pyridinic N-coordinated holes in the graphitic sheets. These sites are ideal for the coordination and "trapping" of precious metals and thus forming a single atom catalyst. These are of great interest to study catalytic processes on a single and uniform site and to severely decrease the precious metals loading for improved catalytic activity. Polydopamine (PDA), a major component of the pigment melanin, transforms with pyrolysis to N-doped carbonaceous graphitic material. The PDA can be formed by the polymerization of a dopamine hydrochloride solution in the presence of molecular oxygen from the air at room temperature. We have used polymerization of dopamine to coat iron-oxide magnetic nanoparticles. However, the coating was not thick enough to prevent the major growth of nanoparticles and their transformation to Fe <sup>3</sup><sub>3</sub>C during the pyrolysis. We overcame this problem by coating the consolidated carbonaceous precursor with the PDA. The

benefit is twofold; the amount of dopamine is severely reduced without impairing the desirable surface properties of the PDA and a significant amount of the iron-oxide nanoparticles remains in the size range that enables efficient heating with an AC magnetic field.

The PDA-coated magnetic nanoclusters were studied as catalyst supports in collaboration with the researchers from University of Trieste, Italy (Prof Paolo Fornasiero). We have demonstrated the essential role of the support used for oxygen reduction reaction (ORR) catalysts based on N-, O-doped nanocarbons, which can drastically change the selectivity of the reduction process, favouring either  $H_2O$  or  $H_2O_2$  as the main product. The catalyst support was made of PDA-coated iron-oxide nanoclusters that were subsequently removed by acid treatment yielding hollow PDA shells. The catalyst switched the ORR process selectivity, despite the fact that the textural and chemical properties were similar to the standard graphitized carbon support. This work highlights the key parameters that tailor the selectivity for the future design of catalysts for ORR applications.

Besides carbon-coated, alumina-coated magnetic nanoclusters are also desirable. In collaboration with the Department for Nanostructured Materials (Dr Andraž Kocjan), we developed a scalable and simple method for the preparation of high-surface-area alumina-coated magnetic nanoclusters. The Ru nanoparticles were deposited onto the nanoclusters using the reduction of a Ru precursor by isopropanol at an elevated temperature. The nanocatalyst was tested in collaboration with the Department of Catalysis and Chemical Reactions Engineering, National Institute of Chemistry (Dr Blaž Likozar and Dr Miha Grilc) in hydrogenation of levulinic acid.

The nanocatalyst showed remarkable activity, however, it deactivated completely after the first run. Using the TEM and X-ray fluorescence spectroscopy, conducted in collaboration with the Department of Low and Medium Energy Physics (Dr Marjan Nečemer), we showed that during the hydrogenation Al and Fe cations partially dissolve and cause detachment of the Ru nanoparticles and precipitation of Al species on the surface of the Ru nanoparticles. The main focus of our current research is shifted to the hydrogenation of non-acidic substrates, such as furfural and Heck condensation.

Frustrated Lewis pairs are compounds where a Lewis acid and base cannot form a classic adduct because of steric hindrance. There are well-known molecular examples and a few solid-state ones. The compounds are interesting

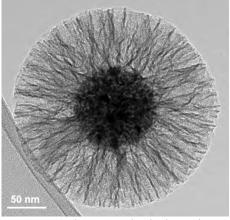


Figure 3: Nanoclusters coated with silica with large, radiallyoriented pores, which enable the loading of an active pharmaceutical substance for magnetic drug delivery.

because the energy of frustration can activate small molecules such as H<sub>2</sub>, CO and CO<sub>2</sub>, which are typically activated by preciousmetals, or on rare occasions, by transition metals. In collaboration with the Department of Inorganic Chemistry and Technology (Dr Gašper Tavčar and Dr Tomaž Skapin) we developed a process for fluorinating the surface layer of the alumina in high-surface-area, alumina-coated magnetic nanoclusters. The formed aluminium fluoride is a remarkably strong Lewis acid because of the coordinately unsaturated surface Al<sup>3+</sup> cations.

We continued our research of novel magnetically-responsive, drug-delivery systems in collaboration with the Faculty of Pharmacy, University of Ljubljana (Prof Petra Kocbek). The controlled assembly of many small superparamagnetic nanocrystals into large nanoclusters is needed for effective magnetic responsiveness. We developed novel one-pot methods for the preparation of the nanoclusters (*i.e.*, magnetic nanocarriers) based on the hot ultrasonication homogenization of a hydrophobic phase containing a nonpolar surfactant into an aqueous phase. The nanocarriers were of spherical shape, with mean hydrodynamic sizes <160 nm, good colloidal stability, and high drug loading. We showed that drug release from such magnetic nanocarriers can be controlled by the type of nonpolar surfactant used for their preparation.

In the frame of another project where we cooperated with researchers from the same faculty, magnetic coreshell-based, drug-delivery systems have been developed. The spherical nanoclusters containing around 80 super-

Magneto-mechanical effect of anisotropic magnetic nanoparticles exposed to a lowfrequency magnetic field was tested in the destruction of cancer cells *in vitro*. paramagnetic iron-oxide nanoparticles were coated with silica with large, radially-oriented pores (Figure 3). The pores in the silica enable loading of an active pharmaceutical substance, while the magnetic core provides magnetic guiding. Our research efforts were focused on the preparation of a delivery system with heat-controlled drug release. The active substance, ibuprofen, was loaded into silica pores and then the pores were closed with the solid 1-tetradecanol. The 1-tetradecanol displays a solid-to-liquid

transformation at temperatures between 38 and 40 °C. We expect that the ibuprofen will be released on a controllable way once the temperature increases above this value.

An important part of the research was devoted to our new concepts of biomedical applications, which are based on the transformation of low-frequency alternating magnetic-field (AMF) energy (1 Hz to 1 kHz) to mechanical energy mediated with anisotropic magnetic nanoparticles. In our project devoted to magneto-mechanical cancer treatment we cooperate with the Faculty for Electrical Engineering (Laboratory for Biophysics - FEE-Biophysics), Laboratory for Bioelectromagnetics - FEE-Magnetics), Faculty of Health Sciences (Laboratory for Clinical Biophysics - FHS), University of Ljubljana, and the Department of Molecular and Biomedical Sciences (B2-JSI). For the magneto-mechanical treatment the anisotropic magnetic nanoparticles are internalized into the cancer cells. When exposed to a magnetic field, the anisotropic magnetic nanoparticle inside the cell directs according to the applied field. The nanoparticle's rotation under the influence of the LF-AMF results in transfer of the force, which is applied to damage the cell interior. Two magnetically different anisotropic nanoparticles are being tested; hard-magnetic hexaferrite nanoplatelets (~50 nm wide and 3 nm thick) and superparamagnetic nanochains (~600 nm long and 80 nm thick). The two types of nanoparticles differ in the mechanism of how they respond to the applied magnetic field. For tracking of the nanoparticles with fluorescence microscopy a fluorescent dye was incorporated into the silica shells of both types of nanoparticles. For the colloidal stability of the nanoparticles in the testing biological fluids, large hydrophilic molecules, e.g., dextran or PEG, were grafted onto the nanoparticles' surfaces. In 2018 we continued testing of the magneto-mechanical effect of the nanoplatelets on giant unilamellar vesicles (GUVs) in cooperation with the FEE. The GUVs represent the simplest model of a cell membrane, which comes into a contact with nanoparticles first. The nanoparticles are adsorbed on the GUV's membrane. Exposure of the GUVs with platelets to the LF-AMF resulted in cyclic fluctuations of the GUV's shape, corresponding to the field frequency or even causes bursting of the GUVs. The analysis of this process gives us basic information on the properties of AMF, which will lead to the maximum magneto-mechanical effect.

The greatest attention was, however, on *in vitro* assessments of the magneto-mechanical effect of the anisotropic nanoparticles on highly invasive breast adenocarcinoma (MDA-MB-231) and cervical adenocarcinoma (HeLa) cancer cells (cooperation with B2-JSI). Biocompatibility of the nanoparticles and cytotoxicity of the magneto-mechanical treatment were evaluated in *in vitro* studies using Presto blue assay and CyQUANT cell proliferation assay. The viability of the cells was assessed with fluorescence microscopy and flow cytometry. Cells were incubated with different concentrations of the nanoparticles and treated with the AMF for a short period of time. The AMF of different amplitude (1 mT, 10 mT) and frequency (2-100 Hz) was tested. As an alternative, a stronger rotating magnetic field (~ 150 mT, 5 Hz) generated by the rotational motion of the permanent magnets was also tested. Without the exposure to the field the cell viability did not decrease significantly, proving that the nanoparticles are non-toxic. After the treatment with the LF-AMF the cell viability decreased significantly for the nanoplatelets, while the effect was less pronounced for the nanochains.

The process of the nanoparticles' internalization in the cells was followed with transmission electron microscopy (cooperation with Institute of Cell Biology, University of Ljubljana, Prof Mateja Erdani Kreft). Surprisingly, the TEM analysis showed a low concentration of the nanoplatelets well dispersed inside endosomes of the cells (Figure 4). In contrast, the nanochains internalized into the cells in much larger concentrations. To find the answer to the question why the nanoplatelets are much more effective in magneto-mechanical destruction of the cells already at very low concentrations of the internalized nanoparticles compared to the nanochains even at high concentrations, we analysed the nanoparticles' rotation under the AMF. In cooperation with Prof Josep Nogués's group from the Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain, the rotational motion of the nanochains exposed to the AMF was experimentally evaluated by following the magneto-optical effect in solvents with various viscosities and in cell suspensions. The collective rotational motion of the transmitted intensity of a laser beam passing through the medium. The analysis of the transmittance variation as a function of the AMF (6 mT) to the high frequencies over 1.5 kHz. At medium viscosity, matching the viscosity of the cell interior, the maximum energy can be transferred at the frequencies around 120 Hz. This experimental result is in agreement with calculations

(a)

performed at FEE-Biophysics. In contrast to the hard-magnetic nanoplatelets, the superparamagnetic nanochains followed the AMF (6 mT) only at low frequencies, up to 20 Hz even in water. At a larger viscosity in the cell interior the nanochains cannot rotate under the AMF. Because of their low magnetic anisotropy, the nanochain more easily reverses their magnetic moment than rotating with the field. The situation is different if we apply a rotating magnetic field.

In parallel to applications in magneto-mechanical treatment, the magnetic nanoparticles can also be used in diagnostics (teranostics) as contrast agents for the different imaging techniques. We cooperated with the Fluorescence Imaging Group, Universidad Autonoma de Madrid, Spain (Prof. Daniel Jaque) in the development of new, high-contrast, multimodal imaging to be used for cardiovascular systems. The high contrast is made possible by the application of the hexaferrite nanoplatelets in intracoro-

<u>0.5 µm</u> <u>0.5 µm</u>

(b)

Figure 4: HAADF (a) and BF (b) STEM image of the nanoplatelets (marked with arrows) internalized into a cell.

nary optical coherence tomography (IC-OCT). Aligning of the nanoplatelets with the field can be used for efficient background removal during the IC-OCT and, at the same time, to obtain intracoronary images by complementary magnetic resonance imaging (MRI). The nanoplatelets provide a negative T2 MRI contrast with very high relaxivity.

Our collaboration with CNRS-IPBS, Toulouse, France (Dr Jelena Kolosnjaj-Tabi), was dedicated to the biological evaluation of magnetic nanochains. We developed conjugated nanochains that can disrupt the extracellular matrix by combined magneto-mechanical and photo-thermal effects. The role of the extracellular matrix is to provide structural and biochemical support to the surrounding cells. Moreover, this three-dimensional network of extracellular molecular assemblies, such as collagen, enzymes, and glycoproteins, contributes to cancerous and infectious disease progression and a resistance to treatment. In cancers, the mechanical properties of the tumour's micro-environment correlate with chemo-resistance and poor cancer patient survival. In bacterial infections, the mechanical properties of bacterial biofilm matrix regulate the physiological activity of the micro-organisms and shelter single or multiple species of microorganisms, keeping them safe from harmful environmental factors, such as desiccation, a host body's immune system, or antibiotics. The magneto-mechanical and thermal approaches involving prospective anisotropic magnetic particles could thus represent a methodological alternative to manage highly desmoplastic tumours or antibiotic-resistant bacterial infections.

We continued the research related to the ferromagnetic suspensions of barium hexaferrite nanoplatelets in liquid crystals (in cooperation with the Department of Complex Matter in the frame of the national research project, leader Dr. Alenka Mertelj). We were involved in the rheological studies of the ferromagnetic liquid-crystal suspensions. Other studies were focused on an understanding of the colloidal interactions in suspensions of the hexaferrite nanoplatelets in isotropic solvents. In parallel we were involved (with the Department of Complex Matter, Faculty of Mathematics and Physics of University of Ljubljana, University of Bayreuth, and Max Planck Institute for Polymer Research) in theoretical studies of magneto-optic dynamics in ferromagnetic nematic liquid crystals.

We established a fruitful collaboration with the Department of Chemistry, University of Cambridge, UK (Prof Jonathan Nitschke) and the Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy (Prof. Silvia Marchesan). We successfully demonstrated the formation of hybrid nanomaterials made of self-assembled tripeptide ((p-aminobenzoyl)-L-Phe-D-Ala-L-Phe-NH<sub>2</sub>) and metal-organic cages. The composite material forms a gel structure that allows for the spatial separation of chemically distinct phases from one solvent system. The hierarchical supramolecular assemblies allow for time- and space-controlled, selective chemical segregation by means of guest

encapsulation. The gel nanostructure is influenced by the presence of the cages, thus providing new means for time-control over diffusion and, as a consequence, the uptake of small molecules. Our future efforts will focus on the extension of this chemical platform to biocompatible materials able to perform time-controlled guest release.

Furthermore, our intense collaboration with the Department of Chemical and Pharmaceutical Sciences, University of Trieste, was continued on the development of magnetic nanostructures conjugated with short peptides and self-assembled fibrillar peptide nanostructures. Controlling the magneto-mechanical effect of the anisotropic magnetic particles on soft and fragile peptide fibrils was our central research interest.

We continued with the research on 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. Based on our previous discovery of the significant dissolution of fluoride-based upconversion nanoparticles (e.g., Ln-doped  $LnF_{2}$  and  $NaYF_{4}$ ) we focused on the prevention/minimization of their dissolution. The most significant dissolution of the Ln-doped fluorides was detected in the presence of phosphate ions due to the strong interaction between the Ln<sup>3+</sup> and Y<sup>3+</sup> ions, resulting in insoluble Ln(Y)-phosphates. We plan to exploit the insolubility of the Ln-phosphates for the protection of the nanoparticle surfaces against their dissolution by a thin insoluble surface Ln-phosphate layer. We started to develop a synthesis procedure for a heterogeneous nucleation of the Ln-phosphate layer. The preliminary experiments were carried out in the frame of an educational EU project SKOZ with the involvement of high-school students from Gimnazija Kranj. The first results suggest that it is crucial to control the kinetics of the phosphate precipitation in order to prevent homogenous, instead of heterogeneous, nucleation of the Ln-phosphates. The work is continuing in cooperation with Vinča Institute from Belgrade in the frame of our bilateral project. Alternatively, we started to study the efficiency of the phosphonate coatings to prevent the dissolution of the upconverting nanoparticles. We focused on tetraphosphonate, ethylenediamine tetra(methylene phosphonic acid), shortly EDTMP, since this ligand can interact with four phosphonate groups. Our first results show significant reduction (approx. by 4 times) of the nanoparticle dissolution with respect to the bare nanoparticles. The dissolution studies are done in cooperation with the Department of Inorganic Chemistry and Technology (Dr Maja Ponikvar-Svet). All the studies were accompanied with a precise optical characterization in cooperation with the Department of Complex Matter (Prof Boris Majaron).

In the frame of a bilateral project (BI-DE/17-19-5) with Bundesanstalt für Materialforschung und prüfung (BAM), Berlin, Germany, and with the Department for Surface Engineering and Optoelectronics (JSI) we are developing a 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 to their large surface-to-volume ratio.

We also continued our research of materials displaying a positive temperature coefficient of resistivity (PTCR). The focus was on composite materials containing a mixture of a conducting phase (metal) and a non-conducting phase (BaTiO<sub>3</sub> ceramics). Due to the dimensional changes during the phase transformation, in the non-conducting phase disconnections occur in the conductive phase that leads to the PTCR anomaly.

#### Some outstanding publications in the past year

- Makovec, Darko, Belec, Blaž, Goršak, Tanja, Lisjak, Darja, Komelj, Matej, Dražić, Goran, Gyergyek, Sašo. Discrete evolution of the crystal structure during the growth of Ba-hexaferrite nanoplatelets. Nanoscale, ISSN 2040-3364, 2018, vol. 10, issue 30, str. 14480-14491, doi: 10.1039/C8NR03815E. [COBISS.SI-ID 315497].
- Gyergyek, Sašo, Kocjan, Andraž, Bjelić, Ana, Grilc, Miha, Likozar, Blaž, Makovec, Darko. Magnetically separable Ru-based nano-catalyst for the hydrogenation/hydro-deoxygenation of lignin-derived platform chemicals. Materials research letters, ISSN 2166-3831, 2018, vol. 6, no. 8, str. 426-431, doi: 10.1080/21663831.2018.1477847. [COBISS.SI-ID 31457575].
- Lisjak, Darja, Mertelj, Alenka. Anisotropic magnetic nanoparticles: a review of their properties, syntheses and potential applications. Progress in Materials Science, ISSN 0079-6425. [Print ed.], 2018, vol. 95, str. 286-328, doi: 10.1016/j.pmatsci.2018.03.003. [COBISS.SI-ID 31275559]

### INTERNATIONAL PROJECTS

- COST TD1402 RADIOMAG; Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy Prof. Darko Makovec
- Cost Office
- The European Upconversion Network From the Design of Photon-Upconverting Nanomaterials to Biomedical Applications Prof. Darja Lisjak Cost Office
- The Development of a Nondestructive Analytical Method for the Screening of Upconverting Nanoparticles Surface Properties Based on Optical Characterization Prof. Darja Lisjak Slovenian Research Agency
- Dynamic Hysteresis in the Study of Magnetic Nanoparticle Efficacy for Hyperthermia Therapy Asst. Prof. Sašo Gyergyek
  - Slovenian Research Agency

 Design and Synthesis of Chemically Stable Luminescent Core-Shell Upconverting Nanoparticles for Bioimaging Prof. Darja Lisjak Slovenian Research Agency

# RESEARCH PROGRAM

1. Advanced inorganic magnetic and semiconducting materials Prof. Darko Makovec

# **R&D GRANTS AND CONTRACTS**

- 1. Nanotheranostics based on magneto-responsive materials Asst. Prof. Slavko Kralj
- 2. Anisotropic magnetic nanoparticles for the magneto-mechanical therapy of cancer Prof. Darko Makovec
- 3. Electrically tunable ferromagnetic liquids Prof. Darja Lisjak
- 4. Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Darko Makovec
- Ministry of Economic Development and Technology 5. JSI's equipment and working space rental by a company Asst. Prof. Sašo Gyergyek Inovine d. o. o.

Dr. Ute Resch-Genger BAM, Berlin, Germany 6.-8. 11. 2018

Elina Andresen, BAM, Berlin, Germany, 4.-9. 11. 2018

Dr. Jelena Papan, Inštitut Vinča, Belgrade, Serbia 4.-8. 9. 2018

Dr. Dragana Jovanović, Inštitut Vinča, Belgrade, Serbia 23.-29. 9. 2018

- VISITOR FROM ABROAD
- 1. Prof. dr. Gertjan Koster, University of Twente, Enshede, Netherlands, 19.-24.5.2018
- Dr. Akira Ando, Department for Materials Development, Murata Manufacturing Co., Kyoto, Japan, 28.6.-1.7.2018
- Anastasia Loginova, LG Technology Center of Moscow, Moscow, Russia, 2.7.2018
   Vera Solodovnichenko, LG Technology Center of Moscow, Moscow, Russia, 2.7.2018

## STAFF

#### Researchers

- 1. Asst. Prof. Sašo Gyergyek
- 2. Asst. Prof. Slavko Kralj
- 3. Prof. Darja Lisjak
- 4. Prof. Darko Makovec, Head
- 5. Dr. Igor Zajc

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Postgraduates

6.

8.

- 6. Tanja Goršak, B. Sc.
- 7. Sebastjan Nemec, B. Sc.
- **Technical and administrative staff** 8. Bernarda Anželak, B. Sc.
- 8. Bernarda Anzelak, B. So

- Igor Zajc, Mihael Drofenik, "Ferroelectric phase-transition-assisted anomaly in the electric resistivity (FPTAA) of lead-free PTC thermistors", *Journal of materials science. Materials in electronics*, 2018, 29, 4, 2868-2873.
- Nerea Sebastián Ugarteche, Darja Lisjak, Martin Čopič, Oleksandr Buchnev, Alenka Mertelj, "Comparison of dynamic behavior of ferroelectric and ferromagnetic nematic suspensions", *Journal of molecular liquids*, 2018, 267, 377-383.
- 10. Sašo Gyergyek, Andraž Kocjan, Ana Bjelić, Miha Grilc, Blaž Likozar, Darko Makovec, "Magnetically separable Ru-based nano-catalyst for the hydrogenation/hydro-deoxygenation of lignin-derived platform chemicals", *Materials research letters*, 2018, **6**, 8, 426-431.
- 11. Darko Makovec, Blaž Belec, Tanja Goršak, Darja Lisjak, Matej Komelj, Goran Dražić, Sašo Gyergyek, "Discrete evolution of the crystal structure during the growth of Ba-hexaferrite nanoplatelets", *Nanoscale*, 2018, **10**, 30, 14480-14491.
- 12. Tilen Potisk, Alenka Mertelj, Nerea Sebastián Ugarteche, Natan Osterman, Darja Lisjak, Helmut R. Brand, Harald Pleiner, Daniel Svenšek, "Magneto-optic dynamics in a ferromagnetic nematic liquid crystal", *Physical review. E*, 2018, **97**, 1, 012701.
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#### **REVIEW ARTICLE**

 Darja Lisjak, Alenka Mertelj, "Anisotropic magnetic nanoparticles: a review of their properties, syntheses and potential applications", *Progress in Materials Science*, 2018, 95, 286-328.

#### PUBLISHED CONFERENCE CONTRIBUTION

1. Sašo Gyergyek, David Pahovnik, Ema Žagar, Alenka Mertelj, Rok Kostanjšek, Miloš Beković, Marko Jagodič, Heinrich Hofmann, Darko Makovec, "Functionalization of iron oxide nanoparticles with methacrylate-based monomers for preparation of nanocomposites", In: Proceedings of the 9th International Conference on Times of Polymers and Composites: From Aerospace to Nanotechnology, 17-21 June 2018. Ishia, Italy, (AIP conference proceedings **1981**) 2018, 020067.

# DEPARTMENT FOR ADVANCED MATERIALS

At the Advanced Materials Department, 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 bulk 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 oxides for electronic applications, ii) antibacterial and piezoelectrical biocompatible materials and iii) heat-insulation materials with improved properties and sustainability.

#### Functional oxides for electronic applications

In the scope of the investigation of phase relations in ternary oxide systems, where new compounds and solid solutions form and exhibit interesting electric properties, we determined high-temperature phase equilibria in  $Bi_2O_2$ -Mn<sub>2</sub>O<sub>2</sub>-Mn<sub>2</sub>O<sub>3</sub> (M = Fe, Ga, Al) at 770-790 °C. The samples were prepared by the wet-precipitation method from soluble precursors in order to achieve good homogenization of the starting compositions. In these systems we Asst. Prof. Matjaž Spreitzer identified, based on microstructural and XRD analyses, the formation of the  $\gamma$ -Bi<sub>2</sub>O<sub>2</sub> solid solution, which contains up to approximately 1.5 % M,O,, at temperatures above 760 °C. A sillenite compound in the system Bi<sub>2</sub>O<sub>2</sub>-Mn<sub>2</sub>O<sub>3</sub> forms a solid solution in the entire concentration range with sillenite compounds in the systems  $Bi_2O_2$ - $M_2O_3$ . In the Bi<sub>2</sub>O<sub>2</sub>-Mn<sub>2</sub>O<sub>2</sub>-Fe<sub>2</sub>O<sub>2</sub> ternary system, a solid solution with the formula BiFe<sub>1</sub> Mn<sub>2</sub>O<sub>2</sub>, where  $0 \le x \le 0.16$ , is stable. We prepared single-phase ceramics based on this solid solution with a suitable sintering regime. We performed preliminary investigations of the preparation and optimization of piezoelectric properties of the ceramics based on the  $50Ba(Zr_{0.2}Ti_{0.8})O_3-50(Ba_{0.7}Ca_{0.3})TiO_3$  system.

Controlling the preferential orientation of anisotropic ferroelectric particles such as plates is of high importance in view of their piezoelectric applications. At the synthesis temperature the majority of ferroelectrics with the ABO<sub>2</sub>-type perovskite crystal structure exhibit a symmetrical structure and therefore do not show the tendency for growth in the anisotropic shape of plates. This thermodynamic constraint is overcome by the topochemical microcrystal conversion (TMC) of appropriate anisotropic template particles into ABO,-type perovskite particles with the preserved shape of the template. A layered Aurivillius-type Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> perovskite was found to be a very appropriate template for the preparation of MTiO<sub>2</sub> (M = Ca, Sr, Ba, Pb) perovskite plates by TMC reactions. The mechanisms of these transformations have been well investigated in molten salt (NaCl/KCl); however, we first observed that Bi<sub>4</sub>Ti<sub>2</sub>O<sub>12</sub> plates transform to SrTiO<sub>4</sub> with the maintained shape also under hydrothermal conditions. In 2018 we investigated the mechanism of this conversion by transmission electron microscopy (TEM). We found that the transformation to  $SrTiO_3$  predominantly starts at the edge of the  $Bi_4Ti_3O_{12}$  plate and continues laterally to the interior of the plate. In the course of this transformation, the converted SrTiO<sub>2</sub> part resembled a mesocrystalline assembly of smaller square-shaped crystallites (50-200 nm), in which negligible remains of Bi were present. Different heterostructural plates, consisting of a Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> interior, surrounded by a SrTiO<sub>3</sub> frame were obtained after various reaction times (Fig. 1a). In the scope of TMC mechanism studies in the molten salt, we investigated the transformation of Bi<sub>1</sub>Ti<sub>2</sub>O<sub>12</sub> plates to complex A-site-substituted perovskite plates of Ba<sub>1</sub>Sr<sub>2</sub>TiO<sub>2</sub>, and Ba<sub>1</sub>Ca<sub>2</sub>TiO<sub>2</sub>. The local piezoelectric d<sub>12</sub> coefficient with a maximum value of 20 pm/V was determined by piezoresponse force microscope for the  $Ba_{1,x}Sr_{x}TiO_{3}$  plates with x = 0.054. We found that ferroelectricity and piezoelectricity vanished for x > 0.175. In contrast to Ba,  $Sr_{a}$  TiO<sub>2</sub> with a solid solubility across the whole concentration range, the Ca content in the transformed Ba<sub>1</sub>  $Ca_{v}$ TiO<sub>2</sub> plates was limited to x < 0.1 and also the remains of Bi were high (> 1 at. %) at the conversion temperature of 900 °C. The tetragonality, expressed as c/a ratio, was found to decrease with the increase of the Ca content. Nevertheless, in addition to the composition, the annealing conditions also influence the degree of tetragonal distortion. The investigations revealed that longer reaction times and higher temperature (1000 °C) worsen the tetragonality, while they did not decrease the Bi remains.

In the scope of the research on energy-harvesting devices that could transform mechanical, thermal and solar energies into electricity, we focused on the development of self-assembled films using BaTiO, (BTO) plates that could be used as the energy-harvesting part of these devices. Interface self-assembly of the BTO plates was attained by dispersing the plates in isopropanol/oil solution, then injecting on the water surface, followed by deposition on flexible ITO/PET substrate by dip coating. We observed that the stability of the self-assembled layer and plates



Head (since 1. 4. 2018):



Head (until 31. 3. 2018): Prof. Danilo Suvorov

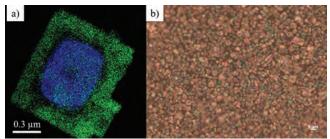


Figure 1: TEM EDS mapping on single plate at the early stage of the topochemical conversion of the Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> plate into the SrTiO<sub>3</sub> plate – blue colour represents bismuth atoms, located mainly at the central part of the nanoplate and the green colour represents strontium atoms, located on the frame and in the central part and b) Self-assembled BaTiO<sub>3</sub> plates on flexible ITO/PET substrate obtained through interface self-assembly.

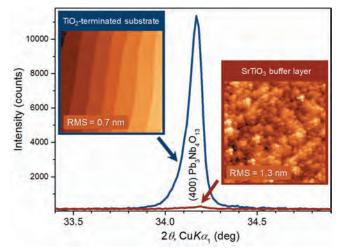


Figure 2: X-ray diffractogram of samples prepared on (i) a TiO<sub>2</sub> terminated STO substrate and (ii) an STO buffer layer. The  $2\theta$  range with the undesired pyrochlore phase ( $Pb_3Nb_4O_{13}$ ) reflection is shown. The insets show the starting surfaces, imaged by means of atomic force microscopy.

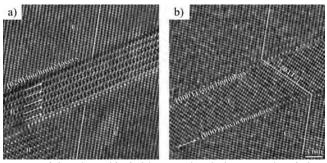


Figure 3: (a) Boehmite-like (B') layers within the host corundum ( $C_1$ ). (b) Recrystallized lamella to corundum in twin orientation ( $C_2$ ).

ordering depend considerably on the dispersion's US agitation time, oil composition and functionalization of the plates' surface. The best results were obtained for the functionalized BTO plates with oleic acid dispersed in the isopropanol-toluene mixture, with a US agitations time of 20 min (Fig. 1b).

The perovskite-type calcium copper titanate  $CaCu_3Ti_4O_{12}$  (CCTO) has an anomalously high dielectric permittivity over a wide range of temperatures and frequencies. This property can be ascribed to various factors; however, none of them properly explain the behaviour. Within our international cooperation we investigated the role of oxygen in the formation of different types and concentrations of defects in the CCTO ceramics. By employing several spectroscopic techniques such as PL, UV–vis, FTIR, and EPR we identified the defect complexation between acceptor centres and neutral, monovalent, and divalent oxygen vacancies, related to the oxygen variation and copper deficiency in the CCTO lattice. We found correlations between the optical and luminescence properties of polycrystalline CCTO ceramics and their dielectric properties. We also established a direct correlation of the defect population and the oxygen partial pressure during the sintering process.

In the pulsed-laser deposition of epitaxial Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-PbTiO<sub>3</sub> (PMN-PT) thin films on different surfaces, such as TiO<sub>2</sub>-terminated SrTiO<sub>2</sub> (STO), SrO, SrRuO<sub>3</sub>, PbZr<sub>1,r</sub>Ti<sub>r</sub> (PZT) in LaNiO<sub>3</sub> (LNO), we found that the surfaces of PZT and LNO enable single-phase growth of PMN-PT, i.e., without pyrochlore inclusions, even if we use targets that do not contain PbO excess. Further experiments showed that the main reason for the enhanced stability of the perovskite phase is the pronounced surface roughness, which enables stronger binding of Pb-based species. In order to prepare high-quality PMN-PT thin films on STO, we modified the surface of the STO single crystals by depositing a homo-epitaxial thin film prepared under specific conditions that ensure the growth of a stoichiometric and simultaneously rough STO layer. This enabled us to significantly improve the phase purity of PMN-PT on STO (Fig. 2), which represents an important step in the fabrication of piezoelectric energy harvesters that operate in the longitudinal mode. Additionally, such a rough STO layer can also improve the integration of other Pb-based functional oxides on Si.

A great research focus was put on the integration of functional oxides with silicon. Alternative routes were explored, including the application of 2D materials, which act as epitaxy-enabling agents. Advanced synthesis and processing methods were used for the surface treatment and several key parameters were identified that influence the quality of the oxide growth. Preliminary results demonstrate the high applicative potential of the studied integration method.

In collaboration with the Institute of Geotechnics, Slovak Academy of Sciences (Košice, Slovakia) we performed nanostructural analyses of mechanochemically synthesized sulphides and selenides. Mechanochemical synthesis is a simple, efficient and environmentally friendly technique for the synthesis of various advanced functional materials. Using techniques of high-resolution electron microscopy we showed that complex sulphides

like kesterite,  $Cu_2 ZnSnS_4$ , which is a promising solar-cell absorber material in thin-film photovoltaics, exhibit a more homogenous chemical composition when prepared from nanosized binary sulphides. The collaboration also related to the synthesis of cobalt selenide,  $Co_9Se_8$ , where it turned out that a Co surplus and a combination of mechanochemistry and thermal annealing in argon is the most efficient approach for the synthesis of this compound with interesting optical and magnetic properties. With researchers from the Sobolev Institute for Mineralogy from Novosibirsk in Russia, we completed a study of defects in large corundum crystals prepared by homo-epitaxial seed growth under hydrothermal conditions. We found that corundum starts to grow by the formation of sectors on the seed surface. On the contacts between the sectors we found 10–30-nm-thick layers of oxyhydroxide phase similar to boehmite lying parallel to the basal planes of the corundum. In the process of dehydration, boehmite topotaxi-

ally recrystallizes to corundum in normal or twinned orientation and the twinned domains are macroscopically expressed as growth defects (Fig. 3).

#### Antibacterial and piezoelectrical biocompatible materials

In the field of the development of biocompatible piezoelectric materials for the electrostimulation of cells or tissues in regenerative medicine, the process of the preparation of piezoelectric independent films of thickness  $\approx 100 \,\mu\text{m}$  from the biodegradable PLLA polymers was optimized by the process of hot pressing and mechanical

stretching of the polymer. The electrical characterization of films confirmed the piezoelectric properties, which are related to the high crystallinity and uniaxial orientation of the polymer chains within the film (Fig. 4a). In order to improve the bioactivity and mechanical properties of the polymer, composites with an inorganic component of calcium hydroxyapatite were prepared. This also improves the hydrophilicity of the film, which contributes to the better interaction of the composite with the biomaterial. We also started with the preparation of PLLA membranes, in the form of distributed nanotubes on a polymeric basis, prepared using the AAO template (Fig. 4b). In this case, a membrane with a high active surface and a rough relief was obtained, which satisfies the conditions for better cell-surface interactions.

Related to the research on new biomaterials, that combine magnetic and antimicrobial properties, the influence of zinc substitution on the physicochemical properties of solvothermally derived cobalt ferrite nanoparticles ( $Co_{(1-x)}Zn_xFe_2O_4$ ; x=0, 0.05, 0.1, 0.3 and 0.5), with the same particle size distribution and amount of capping agent, was investigated. The partial substitution of cobalt ( $Co^{2*}$ ) with zinc ions ( $Zn^{2*}$ ) was proposed in order to tune the magnetic properties of the  $CoFe_2O_4$  and to lower the potential toxicity of the cobalt. The results show that the obtained parti-

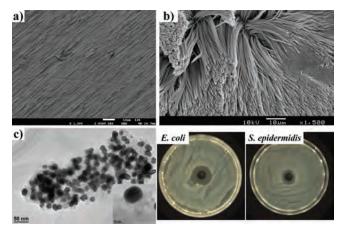


Figure 4: a) Orientation of PLLA chains on the surface of polymer film, b) distributed nanotubes on a polymeric basis, prepared using the AAO template and c)  $Co_{a5}Zn_{a5}Fe_2O_4$ Au nanocomposite and disc diffusion test against E. coli and S. epidermidis.

cles are sphere-like in shape with a mean diameter of  $\sim 5\pm 1$  nm, covered with a complete monolayer of oleic acid, which is covalently bonded to the surface metal atoms. Magnetic measurements show that the particles exhibit superparamagnetic behaviour at room temperature, allowing their use in biomedicine. In addition, we synthesized composites that combine functionalized gold nanoparticles, as an antibacterial component, with zinc-substituted cobalt ferrite nanoparticles, as a magnetic component (Fig. 4c). The prepared composites display antibacterial properties against *E. coli* and *S. epidermidis* and do not cause damage to blood cells, which makes them prospective for further research in biomedicine.

#### Materials for heat-insulation applications

Thermal insulation materials with improved insulation capability, temperature and time stability, and/or improved sustainability directly contribute to the reduction of  $CO_2$  emissions in the construction and building sector. We continued with the investigation of foaming mechanisms of glasses using various standard and custom-designed techniques. The research was focused on the preparation of foamed-glass samples from various waste sources. The foaming additives were selected in accordance with the composition of the glass in order to obtain effective foaming, a high fraction of closed porosity and limited crystallization. The crystallization can impose limitations or even deteriorate the foaming process and foams' properties. By adding specific foaming additives, we were able to tune the composition and foaming process of flat glass to avoid crystallization and prepare a foamed-glass sample with closed porosity, small pore size and low thermal conductivity of 45 mW/(m·K). On the other hand, bottle glass with only minor differences in the composition proved to be much more prone to crystallization. Due to a higher content of transition-metal oxides, the need for the addition of oxidizing agent is much smaller. To develop an effective foaming process for bottle glass we seek for alternative foaming additives to tune the stability of the glass and the surface tension.

In addition to the research on thermal insulation and the mechanical properties of foamed glass, attention is paid to the environmental impact of the product. For this reason, the development aims at the preparation of foamed glass from higher fractions of waste glass in processes that are less energy demanding. The previously developed method for the preparation of foamed glass from cullet in an inert atmosphere was transferred to an air atmosphere, resulting in a low porosity of the products due to the premature reaction of the carbon-based foaming agent with oxygen from the air. By using appropriate additives, the foaming agent can be protected from the atmosphere during heating, thus allowing the formation of a highly porous material. However, additives induce changes in the foaming mechanism. We focused on studying these modified mechanisms in order to enable foaming by a less-energy-demanding process.

#### Characterization of electrical properties

In the scope of electrical properties' measurements the main focus was on the piezoelectric characterization of polymer materials and the measurement of the thermal conductivity of the foamed glass. For the direct measurements of the  $d_{31}$  parameter in polymer films, we adapted our existing  $d_{33}$  meter, while for the thermal conductivity of foamed glass we developed the new vacuum cell for measurements of five samples. The developed cell design is suitable for measurements in the air and in CO<sub>2</sub>. We also continued our work on measurements of the dielectric and ferroelectric properties of bulk ceramics, as well as on temperature-dependent dielectric scans. In addition, we continued with the development of the setup for the electrical characterization of thin films.

In the scope of the M-ERA.NET project **HarvEnPiez** we deal with the synthesis of various defined-shape ferroelectric particles with anisotropic shape (plates, rods) that have a controlled preferential orientation. Their self-assembled structures are proposed for energy-harvesting applications. Since the  $MTiO_3$ -type perovskite particles do not show the tendency for anisotropic growth in the shape of plates and rods, we used the topochemical transformation for their preparation. The main focus is on studying the reaction mechanism of topochemical conversion from  $Bi_4Ti_3O_{12}$  to  $MTiO_3$  (M = Ba, Ca, Sr) and their solid solutions in molten salt and under hydrothermal conditions. The project is a cooperation between Slovenia, Latvia and Romania. The Latvian group is involved in *ab-initio* calculations and modelling of the piezoelectric properties, whereas the role of the Romanian group is in designing and fabricating a piezoelectric device. Funding agency: M-ERA.NET European transnational agency. Coordinator: Dr. Marjeta Maček Kržmanc.

Project **CleanTechBlock II** – Energy Saving Facade Building Component develops and demonstrates a new building block with an improved foamed-glass insulation core and clay brick shells. The thermal insulation testing of a wall segment prepared from 1:1 prototype foamed glass boards revealed an acceptable 10 % mismatch between the material and wall block results. Funding agency: The Energy Technology Development and Demonstration Programme (EUDP) Denmark. Principal investigator: Dr. Jakob König.

Project **CleanTechBlock Basics** – Sustainable Multi-Functional Building Block Basics addresses heat-transfer in foamed glass and demonstrates the adaptability of the CTB wall solution to different climates. Work is focused on the quantification of the different contributions to the effective thermal conductivity in the foamed glass, for which we developed a vacuum cell for probing the thermal conductivity of the prepared open-porous foamed glass. The testing revealed the contributions of solid conduction, gaseous conduction and, for the first time, the radiation contribution to the effective thermal conductivity in foamed glass. The results were used for the validation of the theoretical calculations. The quantification of the different contributions enables us to develop new procedures focused on minimizing the relevant heat-transfer mechanisms. Funding agency: M-ERA.NET European Transnational Agency. Coordinator: Dr. Jakob König.

Applied project **Mineral wool composites with improved insulation properties** was launched to develop a new, innovative preparation procedure for mineral wool composites. The first outputs of the project are theoretical calculations on the thermal conductivity of the composites and experimental validation of the model by measurements performed on test composite samples. This will provide the boundary compositions for the product with targeted properties. Funding agency: Slovenian Research Agency. Coordinator: Dr. Jakob König.

SIOX aims to exploit the rich functionalities of oxides and their heterostructures, which show great promise within the emerging field of oxide electronics. For their implementation, the epitaxial integration of oxides with silicon platforms using industrially appropriate technology is urgently needed, and its development represents the main goal of SIOX. Funding agency: M-ERA.NET European transnational agency. Coordinator: Asst. Prof. Matjaž Spreitzer.

BI-RS/18-19-050 With the Nuclear Institute Vinća (Belgrade, Serbia) we collaborate in the frame of the bilateral project "Synthesis of  $R_2MoO_6$ :REE luminescent nanopowders and their structural characterization by electron microscopy", where we develop novel luminescent nanomaterials for advanced applications. Using a cost-effective, self-initiated and self-sustained synthesis approach we developed thermally and chemically stable  $Eu^{3+}$  activated yttrium molibdate, which can efficiently absorb energy in the near-UV region (324-425 nm) and emit in the red region of the spectrum (611 nm). Funding agency: Slovenian Research Agency. Principal Investigator: Asst. Prof. Nina Daneu.

**BI-FR-PROTEUS**/17-18-007 In collaboration with Géosciences Montpellier we studied twinning in olivine crystals, which occur in ultramafic mantle serpentinites found near Cerro del Almirez in southern Spain in the frame of the bilateral project "Hydratation defects and twinning in silicates". We found that twins in olivine form by dehydration of the precursor mineral clinohumite, which is transformed to twinned olivine in the process of oriented (topotaxial) recrystallization of clinohumite. The results will contribute to a deeper understanding of the recycling of water in the Earth through the formation of protonated defects, which may be the special ingredient in the recipe for plate-tectonics that shapes our planet. Funding agency: Slovenian Research Agency. Principal Investigator: Asst. Prof. Nina Daneu.

BI-RS/18-19-042: "Nanostructured and mesoporous functional materials with accentuated photocatalytic properties under the influence of sunlight" The main aim of this investigation is to prepare functional materials that would exhibit solar-light-driven photocatalytic activity in water-pollutant degradation. The synthesis of the following materials is planned: nanostructured ZnO, ZnO/PEO composites, ZnO/SnO<sub>2</sub> particles, hierarchically structured TiO<sub>2</sub> particles with mesoporous nanostructure and large specific surface area, as well as BaTi<sub>0.9</sub>Sn<sub>0.1</sub>O<sub>3</sub> particles/ceramics. Funding agency: Slovenian Research Agency. Principal Investigator: Asst. Prof. Srečo Škapin.

#### Some outstanding publications in the past year

- Nemanja Aničić, Marija Vukomanović, Tilen Koklič, Danilo Suvorov, "Fewer defects in the surface slows the hydrolysis rate, decreases the ROS generation potential, and improves the Non-ROS antimicrobial activity of MgO", Small, 2018, 14, 26, 1800205.
- Marjeta Maček, Hana Uršič, Anton Meden, Romana Cerc Korošec, Danilo Suvorov, "Ba1–xSrxTiO3Ba1– xSrxTiO3 plates synthesis through topochemical conversion, piezoelectric and ferroelectric characteristics", *Ceram. int.*, vol. 44, no. 17, str. 21406-21414, 2018, doi: 10.1016/j.ceramint.2018.08.198. [COBISS. SI-ID 31620647]
- Urška Gabor, Matjaž Spreitzer, Hana Uršič, Elena Tchernychova, Zoran Samardžija, Wen J. Wu, Danilo Suvorov, "Structural peculiarities of 0.67Pb(Mg1/3Nb2/3)O30.33PbTiO30.67Pb(Mg1/3Nb2/3)O30.33PbTiO3 thin films grown directly on SrTiO[sub]3 substrates", *J. Eur. Ceram. Soc.*, vol. 38, no. 13, str. 4453-44642, 2018, doi: 10.1016/j.jeurceramsoc.2018.06.013. [COBISS.SI-ID 31498279]
- Daniel Diaz-Fernandez, Matjaž Spreitzer, Tjaša Parkelj Potočnik, Danilo Suvorov, "Multi-stage pulsed laser deposition of high quality epitaxial ultra-thin SrTiO[sub]3 on Si substrates", *Appl. surf. sci.*, vol. 455, str. 227-235, 2018, doi: 10.1016/j.apsusc.2018.05.173. [COBISS.SI-ID 31442727]

#### Awards and appointments

- 1. Marija Vukomanović, Danilo Suvorov, Srečo Davor Škapin: Silver medal for the invention of "Functionalized hydroxyapatite/gold composites as 'green' materials with antibacterial activity and the process for preparing and use thereof", 16<sup>th</sup> International Exhibition of Innovations (ARCA 2018), Zagreb, Croatia.
- 2. Sonja Jovanović: Best oral presentation of the 20<sup>th</sup> Conference YUCOMAT 2018, Herceg Novi, Montenegro: "Synthesis of antimicrobial cobalt ferrite/gold nanocomposites".

#### Organization of conferences, congresses and meetings

- 1. Workshop on international project M.ERA-NET "CTB Basics CleanTechBlock Sustainable Multi-functional Building Block Basics", Ljubljana, 18.- 19. 5. 2018
- 2. Info Day on Materials and Technologies within SRIP Factories of the Future & SKD Section for ceramics, Dol pri Ljubljani, 22. 5. 2018
- 3. Workshop on international project M.ERA-NET "HarvEnPiez-Innovative nano-materials and architectures for integrated piezoelectric energy harvesting applications", Ljubljana, 6. 9. 2018

#### Patents granted

- Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, Functionalized hydroxyapatite/gold composites as "green" materials with antibacterial activity and the process for preparing and use thereof, EP2863751 (B1), European Patent Office, 25. 07. 2018.
- 2. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, A method to produce foam glasses, EP2966044 (B1), European Patent Office, 26. 09. 2018.

## INTERNATIONAL PROJECTS

- COST MP1308; Towards Oxide Based Electronics (TO-BE) Asst. Prof. Matjaž Spreitzer Cost Office
- COST CA 17140; Cancer Nanomedicine From the Bench to the Bedside (NANO2CL) Marija Vukomanović Cost Association Aisbl
- Characterization of Structural Defects in Semiconductor ZnO Films Grown by Atomic Layer Deposition (ALD)
   Prof. Danilo Suvorov
   Slovenian Research Agency
- 4. Hydrous Defects and Twinning in Silicates Asst. Prof. Nina Daneu
- Slovenian Research Agency
  Synthesis of Luminescent Nanopowders of Type R2MoO6:REE and Their Structural Characterization by Means of Electron Microscopy Asst. Prof. Nina Daneu Slovenian Research Agency
- Nanostructured and Mesoporous Functional Materials with Enhanced Solar Light Driven Photocatalytic Activity



Asst. Prof. Srečo Davor Škapin Slovenian Research Agency

## **RESEARCH PROGRAM**

1. Contemporary Inorganic Materials and Nanotechnologies Asst. Prof. Matjaž Spreitzer

# **R & D GRANTS AND CONTRACTS**

- Non-traditional isotopes as identifiers of authigenic carbonates 1. Asst. Prof. Srečo Davor Škapin
- Synthesis and characterization of alkali activated foams based on different waste 2. Ásst. Prof. Srečo Davor Škapin
- 3. Piezoelectric Biomaterials for Electro-stimulated Regeneration Marija Vukomanović
- NanoDryCell: Nanoparticle-assisted desiccation of stem cells for the allogeneic cell 4. therapy
- Dr. Martin Štefanič
- Nanoscale investigations of diffusion controlled topotaxial phase transformations in 5. rutile-corundum host systems Asst. Prof. Nina Daneu
- 6. Engineering of oxides on silicon for future electronics Asst. Prof. Matjaž Spreitzer
- Mineral wool composite with improved insulation properties 7. Dr. Jakob König
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) 8.

# VISITORS FROM ABROAD

- Dr. José-Alberto Padron Navarta, Géosciences Montpellier, CNRS, Montpellier, France, 20.12. - 31.12. 2018
- 2. Dr. Wen Yi Tong, University of Liège, Liège, Belgium, 16. - 21.12. 2018.
- Prof. Jiři Hlinka, Czech Academy of Sciences, Prague, Czech Republic, 22. 24.11. 2018. 3. 4. Dr. Smilja Marković, Institute of Technical Sciences of SASA, Belgrade, Serbia, 29.10. 1.11. 2018
- Dr. Dimitriy Zablotsky, Institute of Solid State Physics University of Latvia, Riga, Latvia, 5. 6.9. 2018.
- 6. Dr. Hans Strauven, Belglas BVBA, Brussels, Belgium, 16.8. 2018.
- Dr. Anastasia Loginova, LG Technology Center of Moscow, Moscow, Russia, 2.7. 2018.

## STAFF

#### Researchers

- Asst. Prof. Nina Daneu 1.
- Dr. Jakob König 2.
- Dr. Gertjan Koster 3.
- 4 Dr. Špela Kunej
- 5.
- Dr. Marjeta Maček Kržmanc 6.
- Asst. Prof. Matjaž Spreitzer, Head, since 01.04.18 Prof. Danilo Suvorov, Head, retired 01.04.18
- Asst. Prof. Srečo Davor Škapin 8
- Dr. Marija Vukomanović 9.
- Postdoctoral associate
- 10. Zoran Iovanović
- 11. Dr. Sonja Jovanović

Asst. Prof. Matjaž Spreitzer

- Ministry of Economic Development and Technology
- 9. Cleantech Block II - Energy Saving Cladding
- Dr. Jakob König Eddp (eudp) Energy Technology Development
- 10 HarvEnPiez: Innovative nano-materials and architectures for integratedpiezoelectric energy harvesting applications
  - Dr. Marjeta Maček Kržmanc Ministry of Education, Science and Sport
- 11. CTB Basics: CleanTechBlock-Sustainable Multi-functional Building Block Basics Dr. Jakob König
- Ministry of Education, Science and Sport 12 SIOX: Engineering of silicon-oxide interface using the pulsed-laser deposition technique Asst. Prof. Matjaž Spreitzer
- Ministry of Education, Science and Sport Investigation of NdDyCoCuFe Rare Earth Alloys Alloys and Related Compounds 13. Prof. Danilo Suvorov Urban Mining Company
- Investigation of NdDyCoCuFe Rare Earth Alloys Alloys and Related Compounds 14 Asst. Prof. Matjaž Spreitzer Urban Mining Company

## NEW CONTRACTS

- Development and characterisation of mineral wool fibres Prof. Danilo Suvorov
- Knauf Insulation, d. o. o., Škofja Loka Mineral wool composite with improved insulation properties 2 Dr. Jakob König
  - Knauf Insulation, d. o. o., Škofja Loka
- Dr. Akira Ando, Murata Manufacturing Co. Ltd., Kyoto, Japan, 28.6. 1.7. 2018.
- Prof. Gertjan Koster, University of Twente, Enshede, Netherlands, 5. 12.5. 2018. 9. Dr. Zdenka Bujňáková, Dr. Matej Baláž, Dr. Peter Baláž, Slovak Academy of Sciences 10. (SAS), Bratislava, Slovakia, 2. - 10.5. 2018.

#### Visiting Researchers

- Dr. Daniel Diaz Fernandez, Universidad Autónoma de Madrid, Spain, 1. 10. 2015 -1. 31. 7. 2018
- 2. Dr. Jyoti Prosad Guha, Missoury University of Science and Technology, Rolla, USA, 14.6. - 31.8. 2018.

12. Dr. Martin Štefanič, left 01.10.18 Postgraduates

- 13. Alja Čontala, B. Sc.
- 14. Dr. Urška Gabor
- 15. Uroš Hribar, B. Sc.
- 16. Tjaša Parkelj Potočnik, B. Sc.
- 17. Lea Udovč, B. Sc.
- Technical officers 18. David Fabijan, B. Sc.
- 19. Damjan Vengust, B. Sc.
- Technical and administrative staff
- 20. Vesna Butinar, B. Sc.
- 21. Silvo Zupančič

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#### ORIGINAL ARTICLE

- J. P. B. Silva, J. Wang, Gertjan Koster, Guus Rijnders, R. F. Negrea, C. Ghica, Chandra K. Sekhar, J. Agostinho Moreira, M. J. M. Gomes, "Hysteretic characteristics of pulsed laser deposited 0.5Ba(Zr<sub>0.2</sub>Ti<sub>0.8</sub>)0<sub>3</sub> – 0.5(Ba<sub>0.7</sub>Ca<sub>0.3</sub>)TiO<sub>3</sub>/ZnO bilayers", *ACS applied materials & interfaces*, 2018, **10**, 17, 15240-15249.
- Alja Čontala, Marjeta Maček, Danilo Suvorov, "Plate-like Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> particles and their topochemical conversion to SrTiO<sub>3</sub> under hydrothermal conditions", *Acta chimica slovenica*, 2018, 65, 3, 630-637.
- 3. Li Lin *et al.* (12 authors), "Epitaxial stress-free growth of high crystallinity ferroelectric PbZr<sub>0.52</sub>Ti<sub>0.48</sub>O<sub>3</sub> on GaN/AlGaN/Si(111) substrate", *Advanced materials interfaces*, 2018, **5**, 2, 1700921.
- 4. Bojana Višić, Eva Kranjc, Luka Pirker, Urška Bačnik, Gašper Tavčar, Srečo D. Škapin, Maja Remškar, "Incense powder and particle emission characteristics during and after burning incense in an unventilated room setting", Air quality, atmosphere & health, 2018, 11, 6, 649-663.
- 5. Janvit Teržan, Petar Djinović, Janez Zavašnik, Iztok Arčon, Gregor Žerjav, Matjaž Spreitzer, Albin Pintar, "Alkali and earth alkali modified CuO<sub>x</sub>/SiO<sub>2</sub> catalysts for propylene partial oxidation: what determines the selectivity?", *Applied catalysis. B, Environmental*, 2018, 237, 214-227.
- 6. Depura Palitha Sunil Pushpakumara De Silva *et al.* (10 authors), "Ferroelectric switching dynamics in  $0.5\text{Ba}(\text{Zr}_{0.2}\text{Ti}_{0.8})\text{O}_3 - 0.5(\text{Ba}_{0.7}\text{Ca}_{0.3}\text{TiO}_3)$  thin films", *Applied physics letters*, 2018, **113**, 8, 082903.
- 7. Jun Wang, Guus Rijnders, Gertjan Koster, "Complex plume stoichiometry during pulsed laser deposition of SrVO<sub>3</sub> at low oxygen pressures", *Applied physics letters*, 2018, **113**, 22, 223103.
- Daniel Diaz-Fernandez, Matjaž Spreitzer, Tjaša Parkelj Potočnik, Danilo Suvorov, "Multi-stage pulsed laser deposition of high quality epitaxial ultra-thin SrTiO<sub>3</sub> on Si substrates", *Applied Surface Science*, 2018, 455, 227-235.
- Sara Tominc, Aleksander Rečnik, Zoran Samardžija, Goran Dražić, Matejka Podlogar, Slavko Bernik, Nina Daneu, "Twinning and charge compensation in Nb<sub>2</sub>O<sub>5</sub>-doped SnO<sub>2</sub>-CoO ceramics exhibiting promising varistor characteristics", *Ceramics international*, 2018, 44, 2, 1603-1613.
- Jakob Koenig, Rasmus R. Petersen, Niels Iversen, Yuanzheng Yue, "Suppressing the effect of cullet composition on the formation and properties of foamed glass", *Ceramics international*, 2018, 44, 10, 11143-11150.
- 11. Marjeta Maček, Hana Uršič, Anton Meden, Romana Cerc Korošec, Danilo Suvorov, "Ba<sub>1-x</sub>Sr<sub>x</sub>TiO<sub>3</sub> plates synthesis through topochemical conversion, piezoelectric and ferroelectric characteristics", *Ceramics international*, 2018, **44**, 17, 21406-21414.
- 12. Una Stamenović, Nemanja Gavrilov, Igor A. Pašti, Mojca Otoničar, Gordana Ćirić-Marjanović, Srečo D. Škapin, Miodrag Mitrić, Vesna Vodnik, "One-pot synthesis of novel silver-polyanilinepolyvinylpyrrolidone electrocatalysts for efficient oxygen reduction reaction", *Electrochimica Acta*, 2018, **281**, 549-561.
- 13. Omodara Gbotemi, Sami Myllymäki, Jani Kallioinen, Jari Juuti, Merja Teirikangas, Heli Jantunen, Marjeta Maček, Danilo Suvorov, Marcin Sloma, Małgorzata Jakubowska, "Characterization of PMMA/BaTiO<sub>3</sub> composite layers through printed capacitor structures for microwave frequency applications", *IEEE transactions on microwave theory and techniques*, 2018, **66**, 4, 1736-1743.
- 14. Fabian Burkhardt, Božo Skela, Nina Daneu, Zoran Samardžija, Sašo Šturm, É. Gaudry, Spomenka Kobe, Jean-Marie Dubois, "A new complex ternary phase in the Al-Cr-Sc push-pull alloy", *Journal of alloys and compounds*, 2018, **768**, 230-239.
- 15. Matej Baláž, Nina Daneu, Michal Rajňák, Juraj Kurimský, Michal Hegedüs, Erika Dutková, Martin Fabián, Mária Kaňuchova, Peter Baláž, "Rapid mechanochemical synthesis of nanostructured mohite Cu<sub>2</sub>SnS<sub>3</sub> (CTS)", *Journal of Materials Science*, 2018, **53**, 19, 13631-13642.
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- 17. Martin B. Østergaard, Rasmus R. Petersen, Jakob Koenig, Yuanzheng Yue, "Effect of alkali phosphate content on foaming of CRT panel glass

using  $Mn_3O_4$  and carbon as foaming agents", Journal of non-crystalline solids, 2018, **482**, 217-222.

- 18. Luka Kelhar, Jana Bezjak, Marjeta Maček, Janez Zavašnik, Sašo Šturm, Primož Koželj, Spomenka Kobe, Jean-Marie Dubois, "The role of Fe and Cu additions on the structural, thermal and magnetic properties of amorphous Al-Ce-Fe-Cu alloys", *Journal of non-crystalline solids*, 2018, 483, 70-78.
- 19. Martin B. Østergaard, Rasmus R. Petersen, Jakob Koenig, Michael Bockowski, Yuanzheng Yue, "Foam glass obtained through high-pressure sintering", *Journal of the American Ceramic Society*, 2018, **101**, 9, 3917-3923.
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- 22. Matjaž Spreitzer, Anton Meden, Danilo Suvorov, "High-temperature solid-state reactions in the (1 – x)Na<sub>0.5</sub>Bi<sub>0.5</sub>TiO<sub>3</sub> – xSrTiO<sub>3</sub> system", *Journal of the European ceramic society*, 2018, **38**, 4, 1399-1406.
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- 24. Anderson A. Felix, Matjaž Spreitzer, Damjan Vengust, Danilo Suvorov, Marcelo O. Orlandi, "Probing the effects of oxygen-related defects on the optical and luminescence properties in CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub> ceramics", *Journal* of the European ceramic society, 2018, **38**, 15, 5002-5006.
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methacrylate, gelatin and poly(beta amino ester) crosslinkers", *Polymer* testing, 2018, **68**, 270-278.

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- Goran Durn, Ivan Sondi, Srečo D. Škapin, Marta Mileusnić, Thilo Rennert, Nuša Cukrov, Vedran Rubinić, Stanko Ružičić, "Understanding the (paleo)soils: from palaeoenvironmetal reconstruction to the role of iron oxides and soil organic matter on the formatin of the surface physicochemical properties and the aggregation processes", In: Darko Tibljaš(ed.), *Conference book*, 9th Mid-European Clay Conference - 09 MECC, Zagreb, Croatia [17-21 September 2018], 2018, 116.
- Nikola Zdolšek, Aleksandra Dimitrijevic, Sonja Jovanović, Biljana Šljukić Paunković, Slobodan Gadžurić, Tatjana Trtić-Petrović, "New carbon

materials based on ionic liquids for application in sustainable environmental processes", In: *Proceedings*, Fourth International symposium on corrosion and materials protection, environmental protection and protection against fire, Bar, 18-21. septembar 2018. godine, 2018, 255-264.

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#### INDEPENDENT COMPONENT PART OR A CHAPTER IN A

#### Monograph

1. Gertjan Koster, M. Huijben, Guus Rijnders, "2 - oxide superlattices by PLD: a practical guide", In: Nini Pryds (ed.), Vincenso Esposito (ed.), *Metal oxide-based thin film structures: formation, characterization and application of interface-based phenomena*, (Metal oxides series), 2018, 27-52.

#### PATENT

- 1. Jakob Koenig, Rasmus R. Petersen, Yuanzheng Yue, *A method to produce foam glasses*, EP2966044 (B1), European Patent Office, 26. 09. 2018.
- Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, Functionalized hydroxyapatite/gold composites as "green" materials with antibacterial activity and the process for preparing and use thereof, EP2863751 (B1), European Patent Office, 25. 07. 2018.

#### MENTORING

1. Urška Gabor, *Pulsed-laser deposition of Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>-PbTiO<sub>3</sub> epitaxial thin films:* doctoral dissertation, Ljubljana, 2018 (mentors Danilo Suvorov, Matjaž Spreitzer).

# 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 the extensive use of *in-vivo* models. These have led to the identification of physiological substrates and resulted in a paradigm shift from the concept of proteases as protein-degrading enzymes to proteases as key signalling molecules. Their catalytic activities are precisely regulated, the most important ways being zymogen activation and inhibition by their endogenous protein inhibitors. Any imbalance in this regulation can lead to pathologies such as autoimmune, neurological and cardiovascular disorders, cancer and osteoporosis. However, protease signalling pathways are only Head: partially understood. Currently, only a minor subset of physiological substrates for a limited number of proteases Prof. Boris Turk has been identified, and their physiological regulation is still not well understood.



As one of the leaders in the field, we were invited to write a review paper in one of the most important journals in the field, Trends in Biochemical Sciences. In this article we gave an overview of the progress and current trends in the field of proteases and their application to biomarker discovery and in-vivo imaging.

We have continued with proteomic approaches devoted to the identification of protease specificities and the identification of physiological protease substrates, as well as with small-molecule approaches in order to develop

novel activity-based probes. In collaboration with dr. M. Drag (University of Wroclaw), we used a hybrid combinatorial substrate library (HyCoSuL) approach to obtain specific fluorogenic substrates and an activity-based probe for monitoring cathepsin L activity in the breast-cancer cell line MDA-MB-231. The use of this probe enabled us to distinguish the activity of cathepsin L from that of other cathepsins, particularly cathepsin B, which is abundant and ubiquitously expressed in normal and transformed cell types. Overall, these studies demonstrate that HyCoSuL-derived smallmolecule probes are valuable tools to image cathepsin L activity in living cells. This approach thus enables the evaluation of the cathepsin L function in tumorigenesis and is applicable to other cysteine cathepsins.

Besides mammalian proteases we have focused on bacterial proteases, namely, gingipains. Gingipains are extracellular cysteine proteases of

the oral pathogen *Porphyromonas gingivalis* and its most potent virulence factors. They can degrade a great variety of host proteins, thereby helping the bacterium to evade the host immune response, deregulate signalling pathways, trigger anoikis and, finally, cause tissue destruction. Host cell-surface proteins targeted by gingipains are the key and span three groups of substrates: immune-regulatory proteins, signalling pathways regulators and adhesion molecules. The analysis revealed that gingipains predominantly inactivate their substrates by cleaving them at one or more sites, or through complete degradation. Sometimes, gingipains were even found to initially shed their membrane substrates, but this was mostly just the first step in the degradation of the cell-surface proteins.

In addition, we focused on other bacterial enzymes due to the increasing emergence of antibiotic-resistant strains such as MRSA and VRSA. Therefore, additional pathways essential for the survival of bacteria needed to be explored in order to develop new strategies and new classes of antibiotics. We proposed that Autolysin E (AtlE), from Staphylococcus aureus, is a cell-wall-degrading enzyme that is a potential drug target. It is a member of the glycoside hydrolase (GH) class, enzymes that commonly have either two catalytic residues and hydrolyse their substrates by inverting or retaining mechanisms or one catalytic residue and undergo retaining, substrate-assisted catalysis. Using site-directed mutagenesis studies we have identified Glu138 as the only catalytic residue. Quantum mechanics/molecular mechanics (QM/MM) simulations of the possible reaction pathways suggest that hydrolysis proceeds via a retaining, water-assisted mechanism and an oxocarbenium ion-like transition state. Our results, on the basis of data from a member of the hydrolase GH73 family, support the hypothesis of the presence of an alterna-

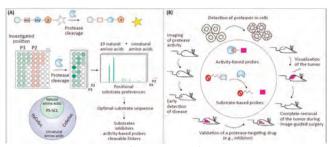


Figure 1. A) Chemical tools for protease profiling. B) In-vivo imaging modalities for laboratory animals.

tive catalytic mechanism in glycoside hydrolases, which can be considered in the design of future AtlE inhibitors. Since we determined the crystal structure of AtlE from *Staphylococcus aureus*, we further used a combination of pharmacophore modelling, similarity search and molecular docking, and identified a series of (Phenylureido)piperidinyl benzamides as potential binders. Surface plasmon resonance (SPR) and saturation-transfer difference (STD) NMR experiments revealed that the selected compounds bind to AtlE in a lower micromolar range. (Phenylureido) piperidinyl benzamides are thus the first reported non-substrate-like compounds that interact with this enzyme and enable the further study of the interaction of small molecules with bacterial AtlE as potential inhibitors of this target.

Another area where we made major progress was the development of drug-delivery systems for cancer treatment. Nanomaterials have become a focus of multidisciplinary research efforts due to their unique physicochemical properties. This includes investigations of their interactions with tumour cells and the stromal compartment of the tumour micro-environment (TME) towards the development of next-generation anticancer therapies. In this work we synthesized aluminium hydroxide mesoporous nanostructures using a modified synthesis method that allowed us to produce a very pure material, without any salt or Al<sup>3+</sup> cations contaminations. The latter is particularly important, since Al<sup>3+</sup> can promote the generation of reactive oxygen radicals and subsequent oxidative damage that could lead to toxicity effects. We have shown that agglomerates of radially assembled Al hydroxide crumpled nanosheets exhibit anti-cancer activity due to their selective adsorption properties and positive charge. This effect was demonstrated in vitro by the decreased proliferation and viability of tumour cells, and further confirmed in vivo in two murine cancer models. Moreover, Al hydroxide nanosheets almost completely inhibited the growth of murine melanoma in vivo in combination with a minimally effective dose of doxorubicin. Our direct molecular dynamics simulation demonstrated that Al hydroxide nanosheets can cause a significant ion imbalance in the living cell perimembranous space through the selective adsorption of extracellular anionic species. This approach to TME dysregulation could lay the foundation for the development of novel anti-cancer therapy strategies.

Part of the work was also devoted to studies related to oxidative stress-induced cell-death mechanisms, which are also relevant for cancer. We have studied the protective effects of four different ROS scavengers, N-acetyl-L-cysteine (NAC),  $\alpha$ -tocopherol and two superoxide dismutase mimetics, n(III)tetrakis(4-benzoic acid)porphyrin chloride, and 4-hydroxy-2,2,6,6-tetramethylpiperidine 1-oxyl (Tempol), on cell death induced by oxidative stress. Four different cell-death models, including menadione-triggered necrosis, staurosporine-induced apoptosis and tumour necrosis factor (TNF)-induced apoptosis and necroptosis, were selected to address this question. We have discovered that menadione-triggered necrosis was completely prevented by the classic ROS scavenger NAC and to a substantial amount by the other scavengers, whereas ROS targeting was found to have a marginal effect on the other cell-death modalities investigated. Despite its side effects at higher concentrations, Tempol was able to substantially prevent TNF-induced apoptosis and to a somewhat lesser extent TNF-induced necroptosis. This is also in agreement with previous suggestions that the use of anti-oxidants cannot completely prevent cell death because ROS are not the only trigger of cell death.

It is worth mentioning that our department has, partially through the help of the Center of Excellence Center for Integrative approaches for Chemistry and Biology of Proteins (CIPKEBIP), which we coordinate, 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. All three platforms are open for external collaborations and several studies resulting from these collaborations have already been published.

In addition, there are numerous other international collaborations with excellent research teams from different countries, including Belgium, Spain, France (through a CEA project), Germany, Sweden, Switzerland, UK, USA, Australia, Hungary and Japan, which resulted in several joint publications.

In addition, we organized a FEBS Workshop on Proteases, Inhibitors and Biological Control in Portorož, which attracts a number of world-class scientists and has become one of the best-known protease-related meetings worldwide. Several members of the department were also invited to give lectures at other international symposia and foreign universities.

#### Some outstanding publications in the past year

- Borišek, Jure, Pintar, Sara, Ogrizek, Mitja, Turk, Dušan, Perdih, Andrej, Novič, Marjana. A water-assisted catalytic mechanism in glycoside hydrolases demonstrated on the Staphylococcus aureus autolysin E. ACS catalysis. 2018, vol. 8, no. 5, str. 4334-4345, doi: 10.1021/acscatal.8b01064.
- Lerner, Marat I., Mikhaylov, Georgy, Tsukanov, Alexey A, Lozhkomoev, Alexandr S, Gutmanas, Elazar, Gotman, Irena, Bratovš, Andreja, Turk, Vito, Turk, Boris, Psakhye, Sergey G., Vasiljeva, Olga. Crumpled aluminum hydroxide nanostructures as a microenvironment dysregulation agent for cancer treatment. *Nano letters.* 2018, vol. 18, no. 9, str. 5401-5410, doi: 10.1021/acs.nanolett.8b01592.

 Vizovišek, Matej, Vidmar, Robert, Drag, Marcin, Fonović, Marko, Salvesen, Guy S., Turk, Boris. Protease specificity : towards in vivo imaging applications and biomarker discovery. TiBS : Trends in biochemical sciences. 2018, vol. 43, no 10, str. 829-844, doi: 10.1016/j.tibs.2018.07.003.

#### Organisation of conferences, congresses and meetings

- 35<sup>th</sup> Winter School on Proteinases and Inhibitors 2018, Tiers, Italy, 28 February to 4 March 2018, coorganizers
- 2. FEBS Workshop 2018 Protease, Inhibitors and Biological Control, Portorož, Slovenia, 8-12 September 2018

#### Patents granted

- 1. Norbert Schaschke, Olga Vasiljeva, Georgy Mikhaylov, Boris Turk, Cathepsin-binding compound bound to a liposome and its diagnostic and therapeutic use, EP2723387 (B1), European Patent Office, 18. 04. 2018.
- 2. Sergey Grigorievich Psakhie, Izraillevich Marat Lerner, Elena Alekseevna Glazkova, Olga Vladimirovna Bakina, Olga Vasiljeva, Georgy Mikhaylov, Boris Turk, Low-dimensional structures of organic and/or inorganic substances and use thereof, US10105318 (B2), US Patent and Trademark Office, 23. 10. 2018.

# INTERNATIONAL PROJECTS

- The Role of Cystatins in Neuroinflamamtion Asst. Prof. Nataša Kopitar – Jerala Slovenian Research Agency
- Cancer management with cathepsin-targeting protein-drug conjugates: application to brain tumor therapies Prof. Boris Turk
- Slovenian Research Agency
- COST BM1307; European Network to integrate Research on Intracellular Proteolysis Pathways in Health and Disease (PROTEOSTASIS) Prof. Boris Turk
- Cost Office
- COST OC-2015; TRANSAUTOPHAGY: European Network of Multidisciplinary Research and Translation of Autophagy Knowledge Prof. Eva Žerovnik
  - Cost Office
- COST CA 15203; Mitochondrial Mapping: Evolution-Age-Gender-Lifestyle-Environment Asst. Prof. Nataša Kopitar – Jerala Cost Office
- COST CA15124; NEUBIAS A New Network of European Bioimage Analysts to Advance Life Science Imaging Asst. Prof. Tina Zavašnik Bergant
- Cost Office
- COST CA15214; An Integrative Action for Multidisciplinary Studies on Cellular Structural Networks Asst. Prof. Nataša Kopitar – Jerala Cost Office

### **RESEARCH PROGRAMS**

- 1. Structural biology
- Prof. Dušan Turk
- Proteolysis and its regulation Prof. Boris Turk

# R & D GRANTS AND CONTRACTS

- 1. Structural insight into iodine metabolism Dr. Ajda Taler-verčič
- Insights into the protein interactions involved in the Potato virus Y potatorelation Prof. Dušan Turk
- Cathepsin X inhibitors impair the resistence of tumor cells to antiprotease therapy Prof. Boris Turk
- Molecular genetic biomarkers and mechanisms of unresponsiveness to biological therapyanti-TNF in patients with chronic immune diseases Prof. Boris Turk
- The role of micro RNA-21 and cathepsins in delayed preconditioning to acute kidney injury
- Prof. Boris Turk
- 6. Inhibition of Staphylococcus aureus cell wall remodeling
- Prof. Dušan Turk Role of legumain in infection and inflammation
- Prof. Marko Fonović 8. Lyposomal Proteases in Semaphorin Signalir
- Lyposomal Proteases in Semaphorin Signaling and Cell Polarity Prof. Boris Turk Icgeb - International Centre for Genetic
- In Vivo Studies of the Potentiating Action of Micro-Mesoporous Powder Nanomaterials Containing Magnetic Iron Oxides Prof. Boris Turk
  - Institute Of Strength Physics and Materials

## VISITORS FROM ABROAD

- 1. Prof. dr. Jiři Neužil, Griffith University, Southport, Qld, Australia, 4-6 April 2018
- 2. Dr. Pal Tod, Semmelweis University, Hungary, 14 May 2018
- Prof. dr. Sandra B. Gabelli, The Johns Hopkins University, Baltimore, Maryland, USA, 15-25 September 2018

#### 5. Prof. dr. Miquel Coll, IRB Barcelona, Spain, 28-30 October 2018

### STAFF

#### Researchers

- 1. Dr. Iztok Dolenc
- 2. Prof. Marko Fonović
- Asst. Prof. Nataša Kopitar Jerala
   Prof Brigita Lenarčič\*
- Prof. Brigita Lenarčič\*
   Abelardo Manuel Silva, B. Sc.
- Abelaluo Maluel Silva, B.
   Prof. Veronika Stoka
- 7 Andrei Šali B Sc
- 8. Prof. Boris Turk. Head
- 9. Prof. Dušan Turk

- 4. Dr. Francesca Coscia, Cambridge Biomedical Campus, UK, 30 September to 3 October 2018
- 10. Asst. Prof. Livija Tušar
  - 11. Prof. Olga Vasiljeva
  - 12. Asst. Prof. Tina Zavašnik Bergant, left 01.04.18
  - 13. Prof. Eva Žerovnik
  - Postdoctoral associates
  - 14. Dr. Miha Butinar
  - 15. Dr. Katarina Karničar
  - 16. Dr. Nataša Lindič
  - Dr. Georgy Mikhaylov
     Dr. Jure Pražnikar\*
- Annual Report 2018



- 19 Dr Vida Puizdar
- 20. Dr. Ajda Taler-Verčič 21. Dr. Aleksandra Usenik
- 22. Dr. Robert Vidmar
- 23. Dr. Matej Vizovišek, left 01.11.18
- 24. Dr. Janja Završnik, left 01.11.18
- Postgraduates
- 25. Monika Biasizzo, B. Sc.
- 26. Dr. Janja Božič, 01.10.18, transferred to Department B3
- 27. Andreja Bratovš, B. Sc.
- 28. Marija Grozdanić, B. Sc.
- 29. Urban Javoršek, B. Sc. 30. Aleksander Krajnc, B. Sc., left 01.05.18
- 31. Jure Loboda, B. Sc. 32
- Dr. Sara Pintar, left 01.07.18
- 33. Tilen Sever, B. Sc.

# BIBLIOGRAPHY

- 34. Mojca Trstenjak Prebanda, B. Sc. 35. Eva Vidak, B. Sc. 36. Miki Zarić, B. Sc. Technical officers Dr. Nežka Kavčič 38. Andreja Sekirnik, B. Sc. 39. Ivica Štefe, B. Sc. Technical and administrative staff 40. Maja Orehek, B. Sc. 41. Dejan Pelko 42. Polonca Pirš Kovačič
- 43. Barbara Vrtačnik, left 04.05.18

Note: \* part-time JSI member

#### **ORIGINAL ARTICLE**

- 1. Jure Borišek, Sara Pintar, Mitja Ogrizek, Dušan Turk, Andrej Perdih, Mariana Novič, "A water-assisted catalytic mechanism in glycoside hydrolases demonstrated on the Staphylococcus aureus autolysin E", ACS catalysis, 2018, 8, 5, 4334-4345.
- 2. Marcin Poreba et al. (11 authors), "Selective imaging of cathepsin L in breast cancer by fluorescent activity-based probes", Chemical science, 2018, 9, 8, 2113-2129.
- 3. Katerina Jazbec, Mojca Jež, Boštjan Smrekar, Simona Miceska, Jasmina Živa Rožman, Urban Švajger, Janja Završnik, Tadej Malovrh, Primož Rožman, "Chimerism and gene therapy - lessons learned from nonconditioned murine bone marrow transplantation models", European journal of haematology, 2018, 100, 4, 372-382.
- 4. Jure Borišek, Sara Pintar, Mitja Ogrizek, Simona Golič Grdadolnik, Vesna Hodnik, Dušan Turk, Andrej Perdih, Marjana Novič, "Discovery of (phenylureido)piperidinyl benzamides as prospective inhibitors of bacterial autolysin E from Staphylococcus aureus", Journal of enzyme inhibition and medicinal chemistry, 2018, 33, 1, 1239-1247.
- 5. Izraillevich Marat Lerner et al. (11 authors), "Crumpled aluminum hydroxide nanostructures as a microenvironment dysregulation agent for cancer treatment", Nano letters, 2018, 18, 9, 5401-5410.
- 6. Samra Hasanbašić, Alma Jahić, Selma Berbić, Magda Tušek-Žnidarič, Eva Žerovnik, "Inhibition of protein aggregation by several antioxidants", Oxidative medicine and cellular longevity, 2018, 8613209.
- 7. Nikolai Engedall, Eva Žerovnik, Alexander Rudov, Francesco Galli, Fabiola Olivieri, Antonio Domenico Procopio, Maria Rita Rippo, Vladia Monsurrò, Michele Betti, Maria Cristina Albertini, "From oxidative stress damage to pathways, networks, and autophagy via microRNAs", Oxidative medicine and cellular longevity, 2018, 4968321.
- 8. Min Pan, Henrik Schinke, Elke Luxenburger, Gisela Kranz, Julius Shakhtour, Darko Libl, Yuanchi Huang, Aljaž Gaber, Miha Pavšič, Brigita Lenarčič, Julia Kitz, Mark Jakob, Sabina Schwenk-Zieger, Martin Canis, Julia Hess, Kristian Unger, Philipp Baumeister, Olivier Gires, "EpCAM ectodomain EpEX is a ligand of EGFR that counteracts EGF-mediated epithelial-mesenchymal transition through modulation of phospho-ERK1/2 in head and neck cancers", PLoS biology, 2018, 16, 9, e2006624.
- 9. Janja Božič, Veronika Stoka, Iztok Dolenc, "Glucosamine prevents polarization of cytotoxic granules in NK-92 cells by disturbing FOX01/ERK/paxillin phosphorylation", *PloS one*, 2018, **13**, 7, 0200757.
- 10. Aljaž Gaber, Seung Joong Kim, Robyn M. Kaake, Mojca Benčina, Nevan J. Krogan, Andrej Šali, Miha Pavšič, Brigita Lenarčič, "EpCAM homooligomerization is not the basis for its role in cell-cell adhesion", Scientific reports, 2018, 8, 13269.

#### **REVIEW ARTICLE**

1. Lorenzo Galluzzi et al. (168 authors), "Molecular mechanisms of cell death: recommendations of the Nomenclature Committee on Cell Death 2018", Cell death and differentiation, 2018, 25, 3, 486-541.

2. Matej Vizovišek, Robert Vidmar, Marcin Drag, Marko Fonović, Guy S. Salvesen, Boris Turk, "Protease specificity: towards in vivo imaging applications and biomarker discovery", TiBS: Trends in biochemical sciences, 2018, 43, 10, 829-844.

#### PUBLISHED CONFERENCE CONTRIBUTION

1. Tjaša Tibaut, Tihomir Tomašič, Vesna Hodnik, Marko Anderluh, Sara Pintar, Marjana Novič, Dušan Turk, "Application of fragment based virtual screening towards inhibition of bacterial N-acetyglucosaminidase", In: Marjan Vračko (ed.), Marjana Novič (ed.), 18th International Conference on QSAR in Environmental and Health Sciences (QSAR 2018), June 11-15, Bled, Slovenia. Pt. 2, (SAR and QSAR in environmental research 29), 2018, 9, 647-660.

### INDEPENDENT COMPONENT PART OR A CHAPTER IN A

#### MONOGRAPH

1. Livija Tušar, Marjana Novič, Marjan Tušar, Jure Zupan, "Structural elucidation", In: Reference module in chemistry, molecular sciences and chemical engineering, Jan Reedijk (ed.), [S. n.]: Elsevier, 2018.

#### PATENT

- 1. Sergey Grigorievich Psakhie, Izraillevich Marat Lerner, Elena Alekseevna Glazkova, Olga Vladimirovna Bakina, Olga Vasiljeva, Georgy Mikhaylov, Boris Turk, Low-dimensional structures of organic and/or inorganic substances and use thereof, US10105318 (B2), US Patent and Trademark Office, 23. 10. 2018.
- 2. Norbert Schaschke, Olga Vasiljeva, Georgy Mikhaylov, Boris Turk, Cathepsin-binding compound bound to a liposome and its diagnostic and therapeutic use, EP2723387 (B1), European Patent Office, 18. 04. 2018.

#### MENTORING

- 1. Katja Bidovec, Role of cathepsin D in TNF $\alpha$  and menadione-induced apoptosis: doctoral dissertation, Ljubljana, 2018 (mentor Veronika Stoka; co-mentor Vito Turk).
- 2. Janja Božič, Role of glucosamine on the localization of cathepsins C and E and cytotoxicity of natural killer cells: doctoral dissertation, Ljubljana, 2018 (mentor Veronika Stoka; co-mentor Iztok Dolenc).
- 3. Nežka Kavčič, Different types of cell death and the role of reactive oxygen species in cell death signalling: doctoral dissertation, Ljubljana, 2018 (mentor Boris Turk).
- 4. Sara Pintar, Structural and biochemical characterization of autolysins from Staphylococcus aureus Mu50: doctoral dissertation, Ljubljana, 2018 (mentor Dušan 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

We have been intensively studying the nose-horned viper (Vipera a. ammodytes) venom proteins that affect the blood-coagulation process-haemostasis. In particular, two such proteins, a serine protease homologue with anticoagulant activity (Vaa-SPH-1) and a serine protease with procoagulant, FVIIa-like activity (SP-10).

Components of the intrinsic blood-coagulation pathway, among them FVIIIa, have been recognized as suitable therapeutic targets to treat venous thromboembolism, the pathological process behind two very serious cardiovascular diseases: deep-vein thrombosis and pulmonary embolism. In collaboration with researchers from the National University of Singapore, the University Medical Center Ljubljana, the North Carolina Agricultural and Head: Technical State University, and Novartis, Basel, Switzerland, we succeeded in concluding and publishing the work Prof. Igor Križaj

in which we described a unique glycoprotein from the nose-horned viper venom, Vaa-SPH-1. This molecule, which is structurally an enzymatically inactive serine protease homologue, exhibits a potent anticoagulant action in human blood (Z. Latinović et al., Thromb. Haemost., 118 (2018), 1713-1728). We demonstrated that one of its targets in the blood-coagulation system is factor VIIIa (FVIIIa) of the intrinsic tenase complex, where it antagonizes the binding of FIXa. Anticoagulants with such characteristics are intensively sought, as they would be much safer for medical applications than the current drugs, which frequently induce excessive bleeding and other complications. Vaa-SPH-1 represents a very promising template to design low-molecularmass FVIIIa-directed anticoagulant substances, based on structural features of the interaction surface between Vaa-SPH-1 and FVIIIa. To this end, we constructed a three-dimensional model of Vaa-SPH-1 bound to FVIIIa and proposed the most appropriate structural elements of Vaa-SPH-1 to constitute small FVIIIa-binding molecules, a potential new generation of anticoagulants (Figure 1). The importance of this work is indicated by its immediate recognition, first in the professional community (e.g., by the journals Gene Therapy Weekly, Atlanta, USA and Medicina danes, Ljubljana, Slovenia), and then also by the general public media. In the case of the latter, the project leader, Professor I. Križaj, has been interviewed by the national Radio (Val 202 - Ime tedna (Figure 2); Radio Slovenia 1 - Aktualno), the national TV (TV Slovenia 1 - Dnevnik and Odmevi) and the commercial TV (POP TV - 24 ur).

The work on Vaa-SP-10, the procoagulant venom serine protease with the FVIIa-like activity, substantially advanced in 2018 and we started with the preparation of a publication.

One of our traditional research topics in the field of toxinology is the study of molecular mechanisms of toxic action of secreted phospholipases A<sub>2</sub> (sPLA<sub>2</sub>) from animal venoms. In particular, we are focused on those endowed with presynaptic neurotoxicity ( $\beta$ -neurotoxins). The knowledge that we are gaining by studying toxic sPLA, s is helping us to discover the pathophysiological roles of orthologous mammalian sPLA,s, for example, their role in the development of neurodegenerative diseases such as Alzheimer's disease.

Ammodytoxin (Atx) is a neurotoxic sPLA, from the venom of the nose-horned viper. The result of its action on the motor neuron is the inhibition of secretion of the neurotransmitter acetylcholine into the synaptic cleft and the flaccid paralysis of skeletal muscle. Among the specific effects of Atx on nerve cells are damaged mitochondria, and the damage inflicted is very similar to that induced by the structurally homologous endogenous group IIA sPLA, when its activity is elevated, as, for example, in the early phase of Alzheimer's disease. Using Atx, we have detected the sPLA, receptor R25 in neuronal mitochondria. We developed the protocol for its purification and identified it as the subunit II of cytochrome c oxidase (CCOX), an essential constituent of the respiratory chain complex. We confirmed CCOX as the first intracellular membrane receptor for sPLA, by the alternative Atx-affinity-labelling of purified CCOX and by demonstrating





Figure 1. The intrinsic tenase complex with Vaa-SPH in place of factor IXa. The human intrinsic tenase consists of FIXa and FVIIIa (grey) complexed on the negatively charged plasma membrane of a platelet. In the intrinsic tenase complex, the atomic coordinates of FIXa were replaced with the coordinates of Vaa-SPH (blue) and docked by High Ambiguity Driven protein-protein DOCKing (HADDOCK) to generate the thermodynamically most optimal structure. The contact area between FVIIIa and Vaa-SPH is zoomed in. Amino acid residues involved in major electrostatic interactions are indicated by large letters, while those contributing less to the interaction, by smaller. The figure is adapted from Z. Latinović et al. (Thromb. Haemost., 118 (2018), 1713-1728).

the encounter of Atx and CCOX in PC12 cells. This discovery suggests the explanation of the mechanism by which  $\beta$ -neurotoxins hinder the production of ATP in poisoned nerve endings. It also provides a new insight into the potential function and dysfunction of an endogenous group IIA sPLA<sub>2</sub> in mitochondria. In 2018, a manuscript

# Animal venoms are a rich source of new substances and molecular tools to improve human and animal health.

describing the first intracellular membrane receptor of an sPLA<sub>2</sub> molecule was prepared and accepted for publication in the esteemed journal Scientific Reports (J. **Šribar** et al., *Sci. Rep.*, (2018), in press).

In the area of  $\text{sPLA}_2$  research, we also succeeded in gaining a new international project (BI-RU/19-20-029). With our Russian partners from

the Laboratory of Molecular Toxinology at the Shemyakin and the Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow, for the next two years we will be studying how endogenous sPLA<sub>2</sub>s modulate functions of nicotinic acetylcholine receptor.

In 2018, we systematically analysed two snake venoms (venomics): one from the nose-horned viper and the other from the very rare Croatian karst viper (*Vipera ursinii*).



Figure 2. Description of an original anticoagulant molecule also attracted the general public. The international research consortium led by Professor I. Križaj discovered and described an anticoagulant protein in the venom of the nose-horned viper with a potent anticoagulant activity in human blood. Due to its unique structure and mode of action, it has a great potential for the development of an innovative drug to treat venous thromboembolism. The discovery echoed in the professional as well as in the general public audience. The latter is reflected also in the selection of the project leader as a name of the week on the national radio Val 202.

To aid improving the current antivenom therapy towards higher specificity and efficiency, and to facilitate drug discovery, we constructed, by combining transcriptomic and proteomic analyses, the most comprehensive library of nose-horned viper venom proteins and peptides. Of particular interest, a transcript coding for a protein similar to P-III SVMPs but lacking the catalytic, MP domain was also found at the protein level in the venom. We started to prepare a manuscript, which will be submitted for publication in 2019.

We determined the proteomic profile of the Croatian karst viper venom and, together with our colleagues from the University of Zagreb, also its biological activities. This venom is much less toxic than that from the nose-horned viper and also the pattern of mice dying due to this venom is different. Experiments suggest the presence of a strong neurotoxic component in the Croatian karst viper venom; however, our studies excluded the presence of basic sPLA<sub>2</sub>s, the only known neurotoxic components in the genus *Vipera* venoms. This suggests the discovery of a novel type of neurotoxic molecule in *Vipera* venoms.

In 2018, we reported together with colleagues from the University Hospital of Split and the University of Split, Croatia, two unique cases of poisoning with the nose-horned viper venom in which, for the first time, thrombocytopenic purpura in patients has been detected (B. Lukšić et al., *Medicine*, 97 (2018), e13737). These unexpected clinical findings were characterized by unusually profound thrombocytopenia of the patients and purpura, observed on the face and thorax of both individuals. In most serious cases, such pathology can be even life threatening if not promptly recognized and treated. This is an important message to clinicians to consider the possibility of such a complication also in the case of nose-horned viper envenomation.

In collaboration with colleagues from the Centre for Clinical Toxicology and Pharmacology, University Medical Centre Ljubljana, we investigated an interesting clinical effect, a profound and transient thrombocytopenia of functional platelets in patients envenomed by the nose-horned viper venom. In thromboembolic diseases, such as myocardial infarction and ischemic stroke, platelets play a pivotal role. Currently used antiplatelet drugs have one common side effect—a decreased count of platelets with an inhibited function. Such a condition represents a high risk of life-threatening haemorrhage, especially in interventional cardiology and angiology employing an antithrombotic approach. Our observation may pave the way to the development of a new group of antiplatelet agents, which will minimize the risk of life-threatening bleeding in the antithrombotic approach in interventional cardiology and angiology, and increase the effectiveness of vessel dilatation and emboli aspiration. To this end, we demonstrated in 2018 that reversible thrombocytopenia in patients after poisoning with the nose-horned viper venom is caused by snake C-type lectin-like proteins (snaclecs). From the venom, we isolated a pool of these proteins and, by using flow cytometry, revealed that such an effect is the consequence of their specific interaction with the platelet GPIb receptor. We also showed that GPIIb/IIa and P-selectin did not express on the membrane of these cells, confirming that the platelets did not undergo the activation.

Last year was also the first one for the Slovenian-Serbian bilateral project BI-RS/18-19-005 ("Characterization of new bacterial enzymes to ameliorate food quality and human health"). Partners exchanged visits in the collaborat-

ing institutions. With colleagues from the Institute of Molecular Genetics and Genetic Engineering, Belgrade, we pursued research activities in three main directions as follows. (1) To determine the specificity of the cleavage of the soybean trypsin inhibitor by the bacterial protease, (2) to analyse high-molecular-mass bacterial proteases and (3) to establish the most appropriate expression system for the preparation of a recombinant snake venom CRISP.

At the end of 2018 we initiated a large research project with the collaboration of two foreign groups, the Department of Biotechnology and Biomedicine from the Technical University of Denmark and the Beijing Genomics Institute from Hong Kong. The major aim of the project is to sequence, assemble *de novo*, annotate and thoroughly analyse the complete *Vipera a. ammodytes* genome.

As experts from the field of toxinology, we have been invited as lecturers at expert meetings and scientific conferences. Most worth mentioning are the invitations to D. Kordiš and I. Križaj to deliver keynote lectures at the 19<sup>th</sup> Congress of the European Section of the International Society on Toxinology, Yerevan, Armenia. We were also invited by the Slovenian journal Medicinski razgledi to prepare a review paper on venomous snakes in Slovenia (V. Leban et al., *Med. razgl.*, (2018), in press).

#### Lipid metabolism and signalling

Our work in this field is focused on identifying the cellular pathways of lipid acquisition and utilization that may be targeted to reduce the resistance of cancer cells to stress. The survival of cancer cells during severe stress depends on the availability of extracellular lipids and on their capacity to synthesize, mobilise or recycle their own intracellular lipids. By studying the ways in which cancer cells use lipids, we aim to reduce their remarkable ability to adapt to the inhospitable tumour microenvironment and thus reduce tumour growth, metastasis and resistance to therapy.

In our recent study (E. Jarc et al., Biochim. Biophys. Acta - Mol. *Cell Biol. Lipids*, 1863 (2018), 247–265) we report on a novel mechanism of lipid droplet-mediated protection of cancer cells against metabolic stress. The study provides evidence for a pro-survival and antioxidant role of lipid droplets that orchestrate unsaturated fatty acid storage and trafficking according to cellular needs (Figure 3). We describe the central role of triglycerides stored in lipid droplets in enabling protection from nutrient limitation, oxidative stress and fatty acid lipotoxicity. By silencing the ratelimiting enzyme in lipolytic lipid droplet breakdown, adipose triglyceride lipase (ATGL), by inhibiting lipid droplet biogenesis and by modulating the unsaturation levels of triglycerides stored in lipid droplets, we show that lipid droplets protect sensitive  $\omega$ -3 and  $\omega$ -6 polyunsaturated fatty acids from oxidation by storing them in the form of inert triglycerides, while concurrently providing fatty acids for mitochondrial energy production, redox homeostasis and cell survival. Our lipidomic analyses performed in collaboration with the group of Dr. Robert Zimmermann from the University of Graz, Austria, revealed that fatty acid lipotoxicity can be modulated in aggressive cancer cells by two complementary mechanisms: (1) PLA<sub>2</sub>induced lipid droplet biogenesis that finely tunes the fatty acyl composition of triglycerides stored within and (2) inhibition of ATGL-mediated lipolysis that leads to the retention of fatty acids within lipid droplets. The lipidomic data was additionally published in full in a separate publication (E. Jarc et al., Data Brief, 18 (2018), 234-240). These findings are important for the emerging field of lipid metabolism in cancer, but they also have wider implications for lipid droplet biology and the regulation of nutrient stress in general, which is relevant in various pathophysiological contexts and diseases.

In our comprehensive review with the title "Lipid Droplets in Cancer: Guardians of Fat in a Stressful World" (T. Petan et al., *Molecules*, 23 (2018), e1941), we focused on recent advances describing the involvement of lipid droplets in the protection against nutrient, lipotoxic and oxidative stress in cancer cells and beyond. We discussed the emerging mechanisms of stress-induced lipid droplet biogenesis, the roles of lipid droplets during stress and the complex bidirectional relationship between lipid droplets and autophagy. Because studies on the role of lipid droplets in cancer are relatively scarce, we have provided a broader overview of lipid droplet func-



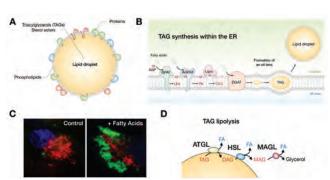


Figure 3. Lipid droplet basics. (A) Lipid droplets are composed of a central hydrophobic core of neutral lipids, mostly triacylglycerols (TAGs) and sterol esters, surrounded by a monolayer of phospholipid molecules, wherein numerous proteins with various functions are embedded. (B) TAG synthesis occurs in the endoplasmic reticulum membrane by sequential addition of fatty acids (FAs) (in their activated acyl-CoA form) to a glycerol-3-phosphate backbone, yielding lysophosphatidic acid (LPA), phosphatidic acid (PA) and diacylglycerol (DAG). These reactions are catalysed by several acyltransferase enzymes, including glycerol-3-phosphate acyltransferases (GPATs), acylglycerol-3-phosphate acyltransferases (AGPATs), and phosphatidic acid phosphatases (lipins). This pathway is also responsible for the synthesis of phospholipids in the cell. The last and committed step in the TAG synthesis cascade is catalysed by the diacyglycerol acyltransferase enzymes (DGATs). (C) Lipid droplet biogenesis is induced in most cells exposed to exogenous FAs. This example shows breast-cancer cells exposed to oleic acid. Lipid droplets (green) were stained with BODIPY 493/503, mitochondria (red) with Mitotracker Red and nuclei (blue) with DAPI and imaged with epifluorescence microscopy. (D) TAG lipolysis occurs by the sequential action of adipose triglyceride lipase (ATGL), hormone sensitive lipase (HSL) and monoacylglycerol lipase (MAGL) and leads to lipid droplet shrinkage and breakdown.

tion in cellular stress in various tissues and pathophysiological settings. Our discussion integrates many of these recently discovered principles of lipid droplet biology that can improve our understanding of the mechanisms that govern cancer-cell adaptability and resilience to stress.

Our work in the field of lipid droplets was well accepted in the scientific community as judged by several invited lectures, most notably at the 14<sup>th</sup> GERLI Lipidomics Meeting – GERLI 40<sup>th</sup> Anniversary on the topic of "Biogenesis and Fate of Lipid Droplets", held in St. Maximin la Saint-Baume, France, where Dr. Petan was invited to present a keynote lecture. Our contributions were also selected for oral presentations at several internationally renowned meetings, including the conference on "Bioactive Lipids – from Chemistry to Biology and Medicine", held in Athens, Greece (T. Petan) and at the 7<sup>th</sup> European Workshop on Lipid Mediators (7EWLM), held in Brussels, Belgium (E. Jarc). Our PhD student Eva Jarc also received a FEBS YTF Travel Grant to attend the FEBS Advance Course "Lipid Dynamics and Membrane Contact Sites", held on the island of Spetses, Greece. Our work was also presented locally at a more public-oriented meeting within the 2<sup>nd</sup> Physiology Day organized by the Slovenian Physiological Society on the occasion of the Nobel Prize for Physiology or Medicine award ceremony and held at the Slovenian Academy of Arts and Sciences, Ljubljana, where Dr. Petan was invited to give a talk on the importance of lipid droplets in cancer.

# High-throughput genetics and functional genomics in yeast *Saccharomyces cerevisiae*; genomics, molecular biology and physiology of extremophilic and extremotolerant yeasts

Polygenic trait analysis and genome editing methods are among the fastest-developing fields in genetics. In a multi-year project on the yeast lipid content analysis, a biotechnologically important polygenic trait, we found three new causative genes for this trait: *PIG1*, *PHO23* and *RML2* (M. Ogrizović et al., unpublished). We also developed

# The genetics and genomics of yeasts for the development of biotechnology.

improvements to the CRISPR-Cas9 method for the yeast genome editing (G. Žun and U. Petrovič, unpublished). In collaboration with the research group of Dr. Gohil from the Texas A & M University, USA, we showed that ethanolamine allows the partial activity of mitochondria in yeast cells that

do not contain cardiolipin (W. Basu Ball et al., *J. Biol. Chem.*, 293 (2018), 10870–10883). This achievement was possible because of our previously developed method for determining the chemogenomic interactions of yeast genes.

Studies of mechanisms enabling survival at extreme values of physico-chemical parameters are often performed on model microorganisms, but they can be complemented by studies of extremophilic and extremotolerant yeasts. In addition to improving our understanding of the ecology of extreme environments, such research importantly expands the possibilities for the exploitation of the substantial biotechnological potentials of microorganisms from such environments. Since these are mostly non-model species and *in vitro* work with them is often non-trivial, we focused primarily on genomic analyses in order to establish a resource for future research. Based on the compara-



Figure 4. Polyextremotolerant black yeasts of the genus Aureobasidium.

tive genomics of extremophilic and extremotolerant yeasts we confirmed the correlation between the ability to grow at high salt concentrations and resistance to oxidative stress in halotolerant species, while the halophilic *Wallemia ichthyophaga* (with a different stress tolerance strategy) did not conform to this observation (C. Gostinčar and N. Gunde-Cimerman, *Genes*, 9 (2018), 143). We studied the glycerol metabolism of two polyextremotolerant yeast species, *Aureobasidium pullulans* and *Aureobasidium subglaciale* (Figure 4) (M. Turk and C. Gostinčar, *Fungal Biol.*, 122 (2018),

63–73). By comparing the genomes of the extremely halotolerant *Hortaea werneckii* we found strong indications of hybridisation within the species (C. Gostinčar et al., *BMC Genomics*, 19 (2018), 364). We used comparative genomics to study the link between opportunistic pathogenicity and poliextremotolerance in 20 species of black yeasts and confirmed the observations with a large-scale phylogenetic analysis (C. Gostinčar et al., *Fungal Fungal Divers*., 93 (2018), 195–213). In collaboration with the group of Dr. Daly from the Uniformed Services University of the Health Sciences, Bethesda, USA, we studied the bioremediation potential of the acidotolerant and radiotolerant yeast *Rhodotorula taiwanensis* (R. Tkavc et al., *Frontiers Microbiol.*, 8 (2018), 2528). In collaboration with the group of Dr. Rodrigues from São Paulo State University, Brazil, we analysed the thermotolerance of proteases of thermotolerant and thermophilic fungi on a genetic level (T.B. de Oliveira et al., *BMC Genomics*, 19 (2018), 152).

#### Evolutionary genomics

*Yarrowia lipolytica* is an oleaginous yeast that can store more than 20% of triacylglycerol (TAG) in its biomass; therefore, it is an attractive host for the production of single-cell oil. Oleaginous microorganisms store large amounts of TAG in intracellular lipid droplets (LDs). In this work we characterized a protein of the oleaginous yeast *Y. lipolytica* that is associated with LD and plays a role in the regulation of TAG storage (G. Bhutada et al., *Biochim. Biophys. Acta – Mol. Cell Biol. Lipids*, 1863 (2018), 1193–1205). This protein is required for the oleagi-

nous phenotype of Y. lipolytica because deletion of the coding gene results in a strongly reduced TAG content of the mutant. Therefore, we named it oleaginicity-inducing LD protein, Oil1. Phylogenomic and phylogenetic analysis demonstrated that Oil1 is a member of the Sps4 family of proteins, which is restricted to the true yeasts (Saccharomycotina). The analysis of secondary structures in fungal LD-associated proteins (Oil1, Sps4, Pet10 and Mpl1) has shown that they consist exclusively of alpha helices. The numbers and the sizes of the helices among the fungal LD-associated proteins vary considerably, and they share no sequence similarity. The analysis of the helices in the Oil1 protein has shown the presence of four amphipathic helices. The 3D structure model of the Oil1 protein shows an extended structure (Figure 5), suggesting bendability of the protein and the interaction of the concave side of the protein with the lipid membrane of the LD. The 3D structure model of the Oil1 protein is most similar to the four-helix bundles, a structure that was also found in perilipins, LDassociated proteins. In summary, our sequence and structure analyses suggested that the Oil1 protein consists mainly of amphipathic helices, which might contribute to the binding of the protein to the LD surface, as it was shown for perilipins.

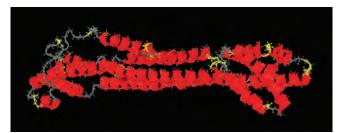


Figure 5. Three-dimensional model of the Oil1 protein. The 3D structure of the yeast Y. lipolytica Oil1 protein was constructed using the I-Tasser server and presented with the Jena3D Viewer. Alpha helices are coloured red, while the unstructured links between them are shown in grey.

Evolutionary, genomic and structure-function analysis of an unusual fungal lipid dropletassociated protein.

#### Other subjects

In 2018 we also participated at several research projects out of the thematic scope of our department. Two collaborative projects resulted in publications in 2018.

As partners in the study of glioblastoma multiforme (GBM), the most common and lethal form of brain tumour, a project led by colleagues from the Medical Faculty of the University of Ljubljana, we participated with the confocal microscopy analysis. To improve the therapy of this tumour and patient outcome, sustained drug delivery to glioma cells is needed, while minimising toxicity to adjacent neurons and glia cells. This may be achieved through an anti-proteomic approach based on nanobodies, the single-domain antigen-binding fragments of heavy-chain antibodies of the camelid adaptive immune system. In this work, we reported on the validation and quantification of a nanobody raised against mitochondrial translation elongation factor (TUFM). Due to its specificity and pronounced inhibitory effect on GBM stem-cell growth, we proposed the use of this anti-TUFM nanobody for GBM *in vitro* immunoimaging and potentially also cancer stem-cell targeting (N. Samec et al., *Oncotarget*, 9 (2018), 17282–17299).

We also contributed to a study of engineering recombinant *Lactococcus lactis* as a delivery vehicle for BPC-157 peptide with antioxidant activities, led by Dr. A. Berlec from the Department of Biotechnology at the Jožef Stefan Institute. Our expertise in flow cytometry and the dynamic analysis of oxidative stress in mammalian cells was crucial for the determination of antioxidant activity of BPC-157, a pentadecapeptide drug candidate for inflammatory bowel disease. In this study, antioxidant BPC-157 was successfully produced by engineered lactic acid bacteria *Lactococcus lactis*, which may be used in the future as a delivery vehicle for this anti-inflammatory peptide in treatments of gastrointestinal inflammation (K. Škrlec et al., *Appl. Microbiol. Biotechnol.*, 102 (2018), 10103–10117).

#### Some outstanding publications in the past year

- Latinović, Z., Leonardi, A., Kovačič, L., Koh, C.Y., Šribar, J., Trampuš Bakija, A., Venkateswarlu D., Kini, R.M. and Križaj, I.: The first intrinsic tenase complex inhibitor with serine protease structure offers a new perspective in anticoagulant therapy. Thromb. Haemost., 118 (2018), 1713–1728
- Jarc, E., Kump, A., Malavašič, P., Eichmann, T.O., Zimmermann, R. and Petan, T.: Lipid droplets induced by secreted phospholipase A<sub>2</sub> and unsaturated fatty acids protect breast cancer cells from nutrient and lipotoxic stress. Biochim. Biophys. Acta – Mol. Cell Biol. Lipids, 1863 (2018), 247–265
- Bhutada, G., Kavšček, M., Hofer, F., Gogg-Fassolter, G., Schweiger, M., Darnhofer, B., Kordiš, D., Birner-Gruenberger, R. and Natter, K.: Characterization of a lipid droplet protein from *Yarrowia lipolytica* that is required for its oleaginous phenotype. Biochim. Biophys. Acta – Mol. Cell Biol. Lipids, 1863 (2018), 1193–1205
- Basu Ball, W., Baker, C.D., Neff, J.K., Apfel, G.L., Lagerborg, K.A., Žun, G., Petrovič, U., Jain, M. and Gohil, V.M.: Ethanolamine ameliorates mitochondrial dysfunction in cardiolipin-deficient yeast cells. J. Biol. Chem., 293 (2018), 10870–10883
- Gostinčar, C., Zajc, J., Lenassi, M., Plemenitaš, A., de Hoog, S., Al-Hatmi, A.M.S. and Gunde-Cimerman, N.: Fungi between extremotolerance and opportunistic pathogenicity on humans. Fungal Divers., 93 (2018), 195–213

#### Awards and Appointments

- 1. Eva Jarc: Youth travel found (YTF) grant for the FEBS Advanced Course, Cambridge, United Kingdom, Federation of European Biochemical Societies, for attending the FEBS Advance course on Lipid dynamics and membrane contact sites, 31August – 7 September 2018, Island of Spetses, Greece.
- Eva Jarc: Scholarship of Slovenian Biochemical Society for young researchers, Ljubljana, Slovenia, Slovenian Biochemical Society, for attending the 7<sup>th</sup> European workshop on lipid mediators, 12 September -14 September 2018, Brussels, Belgium.

#### 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, 19 November and 21 November 2018
- 2. 19<sup>th</sup> European Congress of the International Society on Toxinology, Yerevan, Armenia, 20 September 27 September 2018 (co-organizers)

# INTERNATIONAL PROJECTS

- Gene-Modulatory Role of Human Alpha Satellite DNA: Physiological and Evolutionary Implications Prof. Dušan Kordiš
- Characterization of New Bacterial Enzymes to Ameliorate Food Quality and Human Health Prof. Igor Križaj

# **RESEARCH PROGRAM**

 Toxins and biomembranes Prof. Igor Križaj

# **R&D GRANTS AND CONTRACTS**

1. Applications of aegerolysin-like proteins for detection and eradication of pests Prof. Igor Križaj

- 2. Genetic background of mastitis resistance Prof. Igor Križaj
- 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
- DNA sampling II: a method for identification of directly or indirectly bound proteins at specific loci on bacterial chromosomes Prof. Igor Križaj
- Neurotoxicity or neuroprotection of nanomaterials: the role of biocorona Prof. Igor Križaj
- Crosstalk betwen 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. Anisotropic magnetic nanoparticles for the magneto-mechanical therapy of cancer Prof. Igor Križaj
- Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS Prof. Igor Križaj
- 10. Improved treatment and monitoring of Water Framework Directive priority pollutants Prof. Igor Križaj

# VISITORS FROM ABROAD

- 1. Doc. dr. Miran Brvar, Centre for Toxicology, University Medical Centre, Ljubljana, 30 January 2018
- 2. Dr. Beata Halassy, Centre for Research and Knowledge Transfer in Biotechnology, University of Zagreb, Croatia, 30 January 2018
- Dr. Tihana Kurtović, Centre for Research and Knowledge Transfer in Biotechnology, University of Zagreb, Croatia, 30 January 2018
- Prof. Camelia Tulcan, Banat University of Agricultural Sciences and Veterinary Medicine, Faculty of Veterinary Medicine, Timisoara, Romania, 16 September – 13 October 2018
- Prof. Milan Kojić, Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Serbia, 26 November – 27 November 2018

# STAFF

- Researchers
- 1. Asst. Prof. Cene Gostinčar
- Prof. Dušan Kordiš
   Prof. Jacob Križeći H. 1
- Prof. Igor Križaj, Head
   Asst. Prof. Adrijana Leonardi
- Asst. Prof. Toni Petan
- 6. Prof. Uroš Petrovič\*
- 7. Prof. Jože Pungerčar
- 8. Dr. Jernej Šribar
- Postgraduates
- 9. Ădrijan Ivanušec, B. Sc.
- 10. Eva Jarc, B. Sc.

- Dr. Marija Miljković, Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Serbia, 26 November – 27 November 2018
- Katarina Novović, M.Sc., Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Serbia, 26 November – 27 November 2018
- Dr. Nemanja Stanisavljević, Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Serbia, 26 November – 27 November 2018
- Dr. Goran Vukotić, Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Serbia, 26 November – 27 November 2018
- Dr. Isidoro Feliciello, Ruđer Bošković Institute, Zagreb, Republic of Croatia, 17 December - 18 December 2018
- Prof. Đurđica Ugarković, Ruđer Bošković Institute, Zagreb, Republic of Croatia, 17 December – 18 December 2018
- 11. Ana Kump, B. Sc.
- 12. Mojca Ogrizović, B. Sc., left 01.07.18
- 13. Sabina Ott, B. Sc., left 01.05.18 Technical officer
- 14. Beti Kužnik, B. Sc., left 01.11.18
- Technical and administrative staff
- 15. Igor Koprivec
- 16. Maja Šimaga, M. Sc.

Note: \* part-time JSI member

# BIBLIOGRAPHY

#### **ORIGINAL ARTICLE**

- 1. Janja Zajc, Cene Gostinčar, Metka Lenassi, Nina Gunde-Cimerman, "Stress tolerance of three opportunistic black yeasts", *Acta biologica slovenica: ABS*, 2018, **61**, 2, 15-27.
- Katja Škrlec, Rudolf Ručman, Eva Jarc, Predrag Sikirić, Urban Švajger, Toni Petan, Milica Perišić, Borut Štrukelj, Aleš Berlec, "Engineering recombinant Lactococcus lactis as a delivery vehicle for BPC-157 peptide with antioxidant activities", *Applied microbiology and biotechnology*, 2018, **102**, 23, 10103-10117.
- 3. Eva Jarc, Ana Kump, Petra Malavašič, Thomas O. Eichmann, Robert Zimmermann, Toni Petan, "Lipid droplets induced by secreted phospholipase A<sub>2</sub> and unsaturated fatty acids protect breast cancer cells from nutrient and lipotoxic stress", *Biochimica et biophysica acta. Molecular and cell biology of lipids*, 2018, **1863**, 3, 247-265.
- 4. Govindprasad Bhutada, Martin Kavšček, Florian Hofer, Gabriela Gogg-Fassolter, Martina Schweiger, Barbara Darnhofer, Dušan Kordiš, Ruth Birner-Gruenberger, Klaus Natter, "Characterization of a lipid droplet protein from Yarrowia lipolytica that is required for its oleaginous phenotype", *Biochimica et biophysica acta. Molecular and cell biology of lipids*, 2018, **1863**, 10, 1193-1205.
- Tássio Brito de Oliveira, Cene Gostinčar, Nina Gunde-Cimerman, Andre Rodrigues, "Genome mining for peptidases in heat-tolerant and mesophilic fungi and putative adaptations for thermostability", *BMC* genomics, 2018, 19, 152.
- Cene Gostinčar, Jason Eric Stajich, Jerneja Zupančič, Polona Zalar, Nina Gunde-Cimerman, "Genomic evidence for intraspecific hybridization in a clonal and extremely halotolerant yeast", *BMC genomics*, 2018, **19**, 364.
- Eva Jarc, Thomas O. Eichmann, Robert Zimmermann, Toni Petan, "Lipidomic data on lipid droplet triglyceride remodelling associated with protection of breast cancer cells from lipotoxic stress", *Data in brief*, 2018, 18, 234-240.
- 8. Rok Tkavc, Vera Y. Matrosova, Olga E. Grichenko, Cene Gostinčar, Robert P. Volpe, Polina Klimenkova, Elena K. Gaidamakova, Carol E. Zhou, Benjamin J. Stewart, Mathew G. Lyman, Stephanie A. Malfatti, Bonnee Rubinfeld, Melanie Courtot, Jatinder Singh, Clifton L. Dalgard, Theron Hamilton, Kenneth G. Frey, Nina Gunde-Cimerman, Lawrence Dugan, Michael J. Daly, "Prospects for fungal bioremediation of acidic radioactive waste sites: characterization and genome sequence of Rhodotorula taiwanensis MD1149", *Frontiers in microbiology*, Jan. 2018, **8**, 2528.
- 9. Martina Turk, Cene Gostinčar, "Glycerol metabolism genes in Aureobasidium pullulans and Aureobasidium subglaciale", *Fungal biology*, 2018, **122**, 1, 63-73.

- Cene Gostinčar, Janja Zajc, Metka Lenassi, Ana Plemenitaš, Sybren de Hoog, Abdullah M. S. Al-Hatmi, Nina Gunde-Cimerman, "Fungi between extremotolerance and opportunistic pathogenicity on humans", *Fungal diversity*, 2018, **93**, 1, 195-213.
- 11. Cene Gostinčar, Nina Gunde-Cimerman, "Overview of oxidative stress response genes in selected halophilic fungi", *Genes*, 2018, **9**, 3, 143.
- 12. Writoban Basu Ball, Charli D. Baker, John K. Neff, Gabriel L. Apfel, Kim A. Lagerborg, Gašper Žun, Uroš Petrovič, Mohit Jain Jain, Vishal M. Gohil, "Ethanolamine ameliorates mitochondrial dysfunction in cardiolipindeficient yeast cells", *The Journal of biological chemistry*, 2018, **293**, 28, 10870-10883.
- 13. Boris Lukšić, Svjetlana Karabuva, Joško Markić, Branka Polić, Tanja Kovačević, Julije Meštrović, Igor Križaj, "Thrombocytopenic purpura following envenomation by the nose-horned viper (Vipera ammodytes ammodytes): two case reports", *Medicine*, 2018, 97, 52, 13737.
- 14. Neja Šamec, Ivana Jovchevska, Jure Stojan, Alja Zottel, Mirjana Liović, Michael P. Myers, Serge Muyldermans, Jernej Šribar, Igor Križaj, Radovan Komel, "Glioblastoma-specific anti-TUFM nanobody for invitro immunoimaging and cancer stem cell targeting", *Oncotarget*, 2018, **9**, 25, 17282-17299.
- 15. Zorica Latinović, Adrijana Leonardi, Lidija Kovačič, Cho Yeow Koh, Jernej Šribar, Alenka Trampuš-Bakija, Divi Venkateswarlu, R. Manjunatha Kini, Igor Križaj, "The first intrinsic tenase complex inhibitor with serine protease structure offers a new perspective in anticoagulant therapy", *Thrombosis and haemostasis*, 2018, **118**, 10, 1713-1728.

#### **REVIEW ARTICLE**

1. Toni Petan, Eva Jarc, Maida Jusović, "Lipid droplets in cancer: guardians of fat in a stressful world", *Molecules*, 2018, **23**, 8, 1941.

#### PUBLISHED CONFERENCE CONTRIBUTION

 Janja Zajc, Cene Gostinčar, Maja Ravnikar, Nina Gunde-Cimerman, "Polyextremotolerant yeasts Aureobasidium spp.: antagonistic activity against phytopathogenic fungi", In: Jürgen Köhl (ed.), IOBC-WPRS working group "Biological and integrated control of plant pathogens": preceedings [!] of the XV Meeting "Biocontrol products: from lab testing to product development" at Lleida (Catalonia, Spain) April 23-26, 2018, (IOBC/WPRS bulletin 133), 2018, 177-178.

# DEPARTMENT OF BIOTECHNOLOGY B-3

At the Department of Biotechnology we investigate biological molecules of microbiological, fungal, plant and animal origin using modern biotechnological methods. We would like to apply them for diagnostic and therapeutic purposes in human and veterinary medicine, for plant protection, the preparation of high-quality and safe food and for the protection of the environment, contributing to an improvement in people's health and the environment in which we live. Our research work is focused on the processes of cancer progression and immune response, neurodegenerative processes, the biology of fungi, plant stress response and the search for new biotechnological approaches and products.

Mushrooms are a rich source of unknown and unique proteins with exceptional properties. In 2018 we continued to identify and characterize new proteins from mushrooms. In cooperation with the Biotechnical Faculty of the University of Ljubljana, we were the first to demonstrate the presence of acetylcholinesterase activity in fungi. Acetylcholinesterases are known as one of the catalytically most efficient enzymes and play an important role in Head: the transmission of nerve signals in vertebrates. Cholinesterases have also been described in microorganisms, Prof. Janko Kos protozoa, invertebrates and plants, where they mainly perform various non-neuronal regulatory roles. However, there have been no reports on cholinesterase activity in mushrooms. In our study, a strong cholinesterase activity

was observed in a quarter of 45 tested mushroom aqueous extracts. A surprising variability of these enzymes was shown, and they were not characterized as vertebrate-like cholinesterases. In addition, the presence of acetylcholinesterase inhibitors was demonstrated in a fifth of aqueous extracts, with the wood pinkgill (Entoloma rhodopolium) extract showing an extremely potent inhibitory effect. Inhibitors of cholinesterases are

used in medicine for the treatment of neuromuscular disorders and Alzheimer's disease. In addition, they are used as insecticides, pesticides and nerve agents (for example, sarin). The study confirmed the incredible potential of mushrooms as a source of unknown new natural compounds.

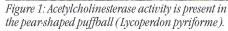
The search for novel antibacterial compounds from mushrooms in cooperation with the Biotechnical Faculty of the University of Ljubliana continued using the food-borne pathogenic and food spoilage bacteria and fungi. Aqueous extracts of various wild mushrooms affected the growth and adhesion of the Grampositive bacteria Listeria innocua and Bacillus cereus, the Gram-negative bacteria Escherichia

coli and Campylobacter jejuni, the yeast Candida albicans and the mould Aspergillus ochraceus. In 2018 our studies in the field of glycobiology focused on the effect of fungal lectins on the biofilm formation of selected pathogenic bacteria. We demonstrated that lectins can either enhance or diminish the biofilm formation of different bacteria. Bacteria in biofilms are particularly resistant to antibiotics and sanitizers, as they are embedded in a self-produced matrix

of extracellular material that protects them from these adverse conditions. Biofilms represent a persistent source of contamination and ensure bacterial survival through industrial foodpreparation processes and in various medical settings. Lectins represent an alternative approach to the prevention of biofilm formation and can contribute to reducing the use of antibiotics. We also investigated the glycosylation profile of the inhibitor of cysteine peptidases cystatin F, which is important for the trafficking of the protein to lysosomal vesicles as well as for the internalization to the immune cells.

Cystatin F is one of the key regulators of immune cytotoxic cells. In these cells it can enter the lysosomes and cytotoxic granules and inhibits the cathepsins C and H, which are the main convertases of progranzymes, the triggers of cell death. Secretory-granule-dependent cytotoxicity is typical for natural killer (NK) cells and cytotoxic T lymphocytes, and consequently we focused our studies on these cell types. Using different cystatin F mutants we have shown that the internalization of both dimeric and monomeric forms of cystatin F leads to a reduction of the activity of cathepsins C and H in recipient cells. The internalization rate of both dimeric and monomeric cystatin F was shown to be governed by their glycosylation pattern. We have also

Cyteine peptidases and their inhibitors modulate the interplay between cancer stem cells, differentiated cancer cells and immune cells in a tumour micro-environment.







Annual Report 2018

demonstrated that cystatin F can be transported to the endosomes/lysosomes of NK cells, resulting in the decreased activity of effector granzymes A and B as well as a lower cytotoxicity towards target cells.

In the previous year we extensively investigated the source of extracellular cystatin F in a tumour microenvironment. In tissue sections obtained from human brain tumours we showed, in collaboration with the National Institute of Biology, that the main source is cancer stem cells, de-differentiated cancer cells and monocytes. We proposed a model of a tumour micro-environment with the interplay between these cells and immune cytotoxic

### The CRISPR/Cas9 system for gene editing was adopted for use in lactic acid bacterium Lactococcus lactis.

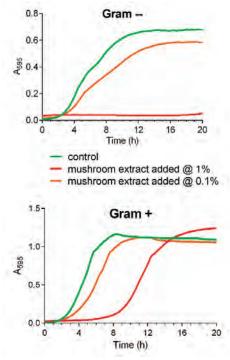


Figure 2: Growth curve. Mushroom extract negatively affects the growth of Gram-negative and Gram-positive bacteria at a very low concentration.

An important feedback loop for the accumulation of TDP-43 in the cytoplasm in patients with frontotemporal dementia has been identified, explaining the mechanism for the occurrence of the disease.

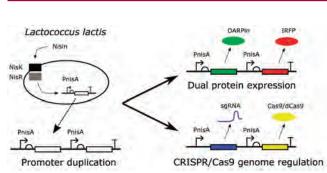


Figure 3. Duplication of the nisin promoter enables the controlled expression of two model proteins (DARPin, IRFP) in L. lactis, while modification of these systems enables the controlled expression/ transcription of elements of CRISPR/Cas9 system (Cas9, sgRNA). cells. In this model cystatin F is an important mediator, causing anergy of cytotoxic cells and consequently lower cancer cell killing. On the other hand, anergic cytotoxic cells with the increased secretion of cytokines, differentiate cancer stem and monocytes to mature cells, which do not express cystatin F and are therefore unable to induce anergy. Differentiated

tumour cells are more sensitive to chemotherapeutics, which might improve the cancer treatment.

As a main transcriptional factor that regulates the expression of cystatin F, c-EBP alpha was identified. Its higher expression is associated with cystatin F in monocytes and cytotoxic cells and CEBP alpha therefore represents a key target for the regulation of cystatin F expression and the function of cytotoxic cells.

In the field of neurobiology we continued with investigations of molecular mechanisms of frontotemporal dementia (FTD) and amyotrophic lateral sclerosis (ALS) with three published articles and another two in the field of Prader Willi Syndrome and disease-associated RNA splicing. We would highlight the publication in the Brain magazine (IF 10.8) about the feedback loop between the TDP-43 protein, dipeptide repetitions, and nuclear transport in the neurodegenerative disease frontotemporal dementia. The work was carried out in collaboration with King's College London. Cytoplasmic accumulation and the aggregation of TDP-43 is the main pathological sign of ALS and FTD. In fruit-fly-based studies that model one genetic form of these diseases, it has been found that the excessive accumulation of soluble fly TDP-43 in cytoplasm causes the pathological accumulation of KPNA2 and KPNA4 proteins, important for nuclear transport, which is even more likely to prevent the transport of TDP-43 to the nucleus. A similar phenomenon was then observed in post-mortem brain patients with frontotemporal dementia. This result has identified an important feedback loop for the accumulation of TDP-43 in the cytoplasm, which could be a mechanism for the occurrence of the disease.

We continued our work on the development of new methods for the genetic engineering of lactic acid bacteria and their potential use for the delivery of therapeutic proteins to the mucosal surfaces. In the field of method development, we prepared a series of plasmid vectors that enable the concomitant controlled expression of two recombinant proteins. We were also the first to prepare a plasmid vector that enables the use of the CRISPR-Cas9 system in the lactic acid bacterium Lactococcus lactis. We confirmed the efficacy on several model genes that were

located either in the genome or in another plasmid. Apart from that, we upgraded the CRISPR-Cas9 system into the CRISPR interference system (CRISPRi) that enables the targeted silencing of selected genes, which is useful in the regulation of signal pathways.

In the field of the development of therapeutic delivery systems, we collaborated with a Czech group (Dr. P. Maly, BIOCEV, Vestec) to develop binders of the p19 subunit of human pro-inflammatory cytokine IL-23 that plays an important role in inflammatory bowel disease and psoriasis. Binders were displayed on the surface of L. lactis and their ability to remove IL-23 from the solution was confirmed. This activity could be useful in decreasing inflammation and we would like to confirm it in future studies in an appropriate animal model.

We have also developed a system for the delivery of the therapeutic peptide BPC-157, whereby we compared the delivery by secretion from bacterial cells, and the delivery by surface display followed by a controlled release mediated by the digestive protease trypsin. BPC-157 is a gastric-stable pentadecapeptide that prevents and treats inflammations of the gastrointestinal tract via its anti-oxidative action. By using custom-developed antibodies and HPLC, we confirmed that a larger quantity of BPC-157 is delivered by using cell secretion from L. lactis. The effective delivery of the peptide was confirmed in a fibroblast cell model, where a statistically significant

decrease in the concentration of reactive oxygen species, important players in inflammation, was observed

The results of the research work at the Department of Biotechnology in 2018 were published in 37 scientific papers in journals with an impact factor. We received three research grants from the Slovenian Research Agency. Dr. Aleš Berlec received the Lapanje plaque award from the Slovenian Biochemical Society for excellent professional achievements. 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. In 2018 two doctoral theses were completed at the department.

#### Some outstanding publications in the past year

- Solomon, Daniel A., Rogelj, Boris, et al. A feedback loop between dipeptide-repeat protein, TDP-43 and karyopherin-[alpha] mediates C9orf72-related neurodegeneration. Brain : journal of neurology, ISSN 0006-8950, [in press] 2018, IF 10,84.
- 2. Pišlar, Anja, Jewett, Anahid, Kos, Janko. Cysteine cathepsins : their biological and molecular significance in cancer stem cells. Seminars in cancer biology, ISSN 1044-579X. [Print ed.], 2018, IF 10,12.
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Figure 4. Frontotemporal dementia associated mislocalization of TDP-43 and KPNA4. In the postmortem brain of FTD patients, the formation of aggregates TDP-43 (green) is noticeable. Aggregates are formed outside the nucleus (white) and are associated with a modified localization of the nuclear transporter KPNA4 (red). (Solomon et al., Brain 2018)

 Kaur, Kawaljit, Perišić, Milica, Ko, Meng-Wei, Safaie, Tahgineh, Kos, Janko, Jewett, Anahid. Natural killer cells target and differentiate cancer stem-like cells/undifferentiated tumors : strategies to optimize their growth and expansion for effective cancer immunotherapy. Current opinion in immunology, ISSN 0952-7915. [Print ed.], 2018, vol. 51, str. 170-180, IF 7,93.

#### Awards and Appointments

1. Aleš Berlec: Lapanje plaque, Ljubljana. Awarded by the Slovenian Biochemical Society for expert and organizational work in society.

#### Organization of conferences and meetings

 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, Ljubljana, 22. 11. 2018

### INTERNATIONAL PROJECTS

- Pathological Mechanisms of TDP-43 in Amyotrophic Lateral Sclerosis and Frontotemporal Dementia Prof. Boris Rogeli
  - Slovenian Research Agency
- Regulation of Cytotoxicity of "Super Charged" Natural Killer Cells with Cystatin F Prof. Janko Kos Slovenian Research Agency
- ALS and FTD Relevant Characterization of In Vivo Protein Interactors of FUS Prof. Boris Rogelj Slovenian Research Agency

## RESEARCH PROGRAM

1. Pharmaceutical Biotechnology: Knowledge for Health Prof. Janko Kos

# R & D GRANTS AND CONTRACTS

1. Evaluation of possible harmful effects of nanoparticles and underlying mechanisms -

from physico-chemical and in vitro toxicity characterisation to innate immune system activation

- Prof. Boris Rogelj
- 2. Nucleart transport defect in neurodegenerative diseases Prof. Boris Rogelj
- Cathepsin X inhibitors impair the resistence of tumor cells to antiprotease therapy Prof. Janko Kos
- Pathogenic role of paraspeckle-like nuclear bodies in neurodegenerative diseases ALS and FTD Prof. Boris Rogelj
- Inhibition of cathepsin X activity as a novel strategy for the treatment of Parkinson's disease
  - Prof. Janko Kos Targeting Campylobacter
- 6. Targeting Campylobacter adhesion in the fight against antimicrobial resistance Dr. Jerica Sabotič
- Targeting, imaging and treating of colorectal cancer with safe theranostic bacteria Asst. Prof. Aleš Berlec
   Phase transitions in systems of nucleotide repeat expansions associated with
- Phase transitions in systems of nucleotide repeat expansions associated with neurodegenerative diseases Prof. Boris Rogelj
- Lactic Acid Bacteria-Mediated Intestinal Delivery of Novel Therapeutic Protein Binders Derived from Scaffold of Albumin-Binding Domain Asst. Prof. Aleš Berlec ZRC SAZU

## VISITORS FROM ABROAD

 Jakub Nowak, Nanotemper Technologies GmbH, Munich, Germany, 1 March 2018
 Lior Levy, M. Sc., Faculty of Biotechnology and Food Engineering, Israel Institute of Technology, Haifa, Israel, 10 June – 15 June 2018

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- 8. Dr. Ana Mitrović
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- 10. Dr. Anja Pucer Janež

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- 1. Janko Kos, Milica Perišić, Mateja Prunk, Jerica Sabotič, Esmeralda Dautović, Anahid Jewett, "Cystatin F as a regulator of immune cell cytotoxicity", *Cancer immunology and immunotherapy*, 2018, **67**, 12, 1931-1938.
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- 3. Katja Škrlec, Surface display of evasins and bepecin on the bacteria Lactococcus lactis NZ9000 and Lactobacillus salivarius ATCC 11741 and evaluation of their anti-inflammatory action: doctoral dissertation, Ljubljana, 2018 (mentor Aleš Berlec).

# DEPARTMENT OF ENVIRONMENTAL SCIENCES 0-2

The Department of Environmental Sciences focuses on the interweaving of the physical, chemical and biological processes that shape our environment as well as humans and their activities. Our research is interdisciplinary and multidisciplinary and takes place in several areas, such as environmental analytical chemistry, biogeochemical cycles, microbial ecology, environment and health, environmental technologies, risk and environmental assessment, and environmental monitoring. We also work on the development of technical solutions for environmental problems and environmental management. 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

The role of trace elements and their impact on the environment and living organisms depends not only on their total concentration but also on the chemical forms in which they are present. Our research is oriented to the Head: development of new analytical procedures for the speciation of elements like Al, As, Cr, Se, Sn, Br, Pt, Ru, Ni, V, Zn Prof. Milena Horvat etc. in environmental, food and biological samples.

In the field of elemental speciation, a procedure was developed for leaching total Cr(VI) from sediments based on a hot alkaline extraction. The use of enriched stable isotopes allowed an accurate determination of Cr(VI) by speciated isotope dilution inductively coupled plasma mass spectrometry (ID-ICP-MS). A new simple, reliable and sensitive analytical method requiring only 1 mL of human serum for a determination of six polybrominated diphenyl ethers (PBDEs) congeners (BDE 28, BDE 47, BDE 99, BDE 100, BDE 153, BDE 154) by gas chromatography (GC)-ICP-MS was developed. Due to its simplicity, sensitivity, reliability and the small amount of sample needed for the analysis, it can be used for biomonitoring purposes.

In order to quantify the accumulation of AgNPs in placental tissue, we tested two sample preparation techniques, alkaline and enzymatic treatment, followed by spICP-MS analysis. We showed that the method using enzymatic tissue treatment is efficient for a determination of mass and number concentration as well as the size distribution of AgNPs in human placental tissues.

An efficient nanomaterial with a 2D structure, high surface area, low cost and metal free was successfully prepared. It is based on graphitic carbon nitrite (g-C3N4) and graphene oxide (GO), which shows very promising results with respect to selectively trapping the Hg(II) present in impinger solutions.

A method for the determination of Sr-90 with the separation based on extractive chromatography and measurements by a liquid scintillation counter with a novel calibration procedure was developed and compared with the traditional method utilizing separation based on fuming nitric acid and measurements on a proportional counter. The developed method enables comparable results and significantly reduces the time and effort needed for the analysis and will be implemented in the future for routine analysis for customers.

Within the framework of the SRA project Non-traditional isotopes as identifiers of authigenic carbonates we developed a procedure for the determination of uranium isotope ratios using MC-ICP-MS. Different strategies for uranium separation from matrix elements were studied in terms of chemical recovery and fractionation. An optimal procedure has been selected and tested on water samples from a karstic aquifer of the Ljubljanica River.

A Rb-Sr radiometric dating method by the MC-ICP-MS has been implemented and optimised. It has been applied for the absolute dating of gneiss from Pohorje, as well as for the magmatic rock from Puerto Angelo, Mexico

The Infrastructure for promoting Metrology in Food and Nutrition (METROFOOD-RI) was successfully included as a new distributed Research Infrastructure on the ESFRI Roadmap. The activities to establish the ERIC status started this year with the JSI being the coordinator of the Slovenian Joint Research Unit.

The implementation of the EMIR SIRS project Metrology for Stable Isotope Reference Standards is in full operation by evaluating the uncertainity of developed new reference CO, gas for determining the isotopic composition of carbon and oxygen. In the framework of the MercOx EMIPR project, we studied the selectivity of different matrices for the separation of elemental and oxidized Hg in the air and liquids.

In the field of interlaboratory comparisons and the development of reference materials, (1) we started with the development of an initial set of calibrated and properly stored RMs for analyzing stable isotopes in vegetable-



oil, honey and cereal samples, and (2) organizing an interlaboratory comparison to determine trace elements in mushroom samples.

In cooperation with CENAM (Mexico), we successfully completed the key study CCQM-K127 Contaminant and other elements in soil, which allowed the entry of new CMCs (calibration and measurement capacities) in the field of chemistry into the KCDB database of the International Bureau for Weights and Measures - Bureau International des Poids et Mesures (BIPM). In 2018, using k0-INAA, ICP-MS and CVAAS, we participated in the characterization of new reference materials ERM-BB185 Bovine liver and ERM-CE101 Fish tissue prepared by the Joint Research Centre in Geel (JRC-Geel), Belgium.

#### Biogeochemical cycles and climate change

Our research focuses on the study of biological, geological and chemical factors that are involved in the cycling of water and chemical elements (light elements: C, N, S, O, H; metals and metalloids: Hg, Cd, Pb, As, Se) in various environmental compartments at the scales of molecules to watersheds. We develop and employ chemical and biological techniques to follow elements' speciation, transformation and isotopic fractionation, including the use of stable and radioactive isotopes as tracers. Our goal is, in cooperation with the wider medical and public health research, to provide an insight into the source-pathway-receptor-consequences relationships.

The Group of Organic Analysis has continued to research the occurrence and cycling of pharmaceutical and personal care products and industrial compounds that have an endocrine-disrupting effect in environmental and wastewaters. During this period, we developed a multi-residue method for determining 48 compounds of emerging concern (CEC: pharmaceuticals, UV filters, preservatives, industrial chemicals etc. and their transformation products) in surface and wastewaters in Slovenia and Croatia. The results showed, besides the common CEC, also the presence of bisphenol analogues and diclofenac transformation products in waste and/or surface waters for the first time. An environmental risk assessment based on risk quotients (RQs) showed that despite low concentrations, two UV-filters (oxybenzone and dioxybenzone), one estrogen (estrone) and one antimicrobial agent (triclosan) were shown to pose a medium-to-high environmental risk. We also synthesised and tested new molecularly imprinted polymers (MIPs) for extracting sertraline and its degradation products and tested their application in the field of environmental analysis and environmental technologies. In the area of non-target analysis, we examined the degradation of sertraline in surface water under the influence of real and simulated solar light. We developed a method for LCMS determination of sertraline transformation products in surface water and determined the occurrence of these compounds in Slovenian rivers.

Work also continues on the treatment/removal of bisphenols in algal-bacterial bioreactors at wastewaterrelevant concentrations in laboratory-scale, batch-fed reactors. This is a collaborative project with the Faculty of Health Sciences, University of Ljubljana. Our aim is to assess the removal (degradation, sorption) of bisphenols from the aqueous phase and their sorption/bioaccumulation in biomass. For this purpose, we have been developing analytical methods to analyse the aqueous phase and algae biomass. The produced algal biomass could also be rich in nutrients and oils, presenting opportunities for reuse. The aim is to evaluate the use of algae as an alternative treatment process together with the possibility of using the algae as an alternative feed source and in other applications from the standpoint of bisphenols content. In parallel, we have also been studying the biological and UV removal of bisphenols from wastewaters in bench top reactors. The aim was to assess their stability, removal mechanism (degradation, transformation, sorption hydrolysis) and formation of stable transformation products using model bisphenol compounds. The results show that bisphenols generally do not hydrolyze in water, are stable in different matrices under test conditions and are efficiently removed by biological treatment. Currently, independent biodegradation experiments in batch reactors have been run with the emphasis theing o apply nontarget analysis (collaboration with University of Antwerp, Belgium) and identify stable transformation products formed from model bisphenols. Our photodegradation experiments consisted of using 1) direct photolysis (UV), 2) cyclodextrin-enhanced photolysis and 3) photo-Fenton reaction in a bench-top UV reactor. Results showed that in all cases degradation follows pseudo-first-order kinetics and the removal efficiency of bisphenols depends on

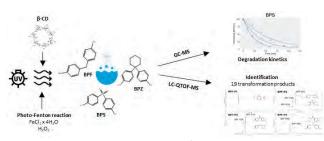


Figure 1: Direct and indirect photolysis of bisphenol alternatives

the applied process. The photo-Fenton reaction resulted in the shortest half-lives. In addition, we have identified eleven novel transformation products. Part of the research results were realized during a two-month secondment to the University of Antwerp, Belgium, organised within the MASSTWIN project. Much effort has also gone into constructing a GC-MS /MS library of derivatized CEC. Once complete, this library will be valuable in testing the performance of software tools designed for identifying CEC compounds in the environment.

The research performed within the GLOBAQUA project includes a geochemical and modelling approach to studying surface-groundwater

interactions and pollution sources of nitrates in the Ljubljansko polje aquifer system. A comprehensive numerical modeling of the steady and transient state of groundwater flow using FEFLOW, which was coupled with MIKE 11 and WaSiM software, was used for modeling the Sava River water flow and percolation. This comprehensive modeling framework was also used to predict the groundwater and surface-water behavior for the period from 2036 to 2065. This period was defined based on climate projections using the three regional climate models provided through the EURO-CORDEX initiative. Modeling shows that the Ljubljansko polje will retain sufficient water capacity and will not suffer due to water scarcity in the period 2036–2065.

The dual isotopic approach using the nitrogen and oxygen of nitrate was applied to identify the sources of nitrates in the Ljubljansko polje aquifer. Based on an isotope-mixing model, three sources of nitrate were identified: atmospheric deposition, fertilizers and soil nitrogen. The data indicate that the main sources of high-nitrate concentrations in groundwater are from fertilizers and sewage-manure (comprising up to 64%). Such levels occurred

in the Hrastje and Kleče 11 wells where precipitation is the main source of groundwater. Nitrate derived from atmospheric deposition accounted for approximately 10% of the nitrate in the groundwater.

Furthermore, the spatial distribution of  $\delta^{18}$ O in precipitation over the Sava River Basin (SRB) was mapped based on the long-term weighted mean annual  $\delta^{18}$ O values and established relationship with various geographical controls (latitude, longitude and altitude). The modelled  $\delta^{18}$ O values in precipitation agree with the measured values in the surface river water at different locations, indicating that the spatial variation in the isotopic composition of precipitation is the dominant factor controlling surfacewater isotope ratios over the SRB.

Special attention was paid to the study of the carbon cycle, which helps us to better understand natural  $CO_2$  sinks and sources and their responses to different environmental changes. The Gulf of Trieste was selected as a case study. The measurements of parameters that describe the carbonate system (pH, T, S, total alkalinity) were performed every two weeks at the oceanographic buoy Vida. It was found that the average temperature vs. biological production ratio (T/B) was 1.74, indicating that the temperature

effect prevails over biological production in controlling the  $CO_2$  dynamics within the Gulf of Trieste. However, it was found that during the summer the changes in  $pCO_2$  were also influenced by biological processes such as phytoplankton uptake and the degradation of organic matter, whereas degassing of  $CO_2$  was not observed. The influence of anoxic conditions on carbon cycling in the Gulf of Trieste was also investigated involving systematic sampling at different locations and water depth in September. This research was perfomed in cooperation with OGS from Italy. The evaluation of the results is still in progress.

In the *water cycle*, snowmelt plays a crucial role in the runoff and recharge of groundwater. While stable isotopes of O and H in water have been standard tools in hydrology for decades, their fractionation during snowmelt and estimation of the contribution of snowmelt to surface runoff and groundwater are still not well understood. Within the IAEA-coordinated international project we tested the efficiency of modified passive capillary snowmelt samplers (PCS) and determined the optimal samplers setup.

In the framework of *paleoclimate research*, a high-resolution O isotopic record in a stalagmite from Pisani rov in Postojna cave was analysed and compared to the long-term precipitation isotope record. To estimate the influence of moisture sources of an isotope composition of precipitation, back trajectory analyses were computed for the days with precipitation in the Postojna area and the moisture uptake locations were identified along these trajectories using standard hydrometeorological formulation. The results showed that the moisture sources do not have a significant impact on the O isotope composition of the precipitation.

It is suggested that the recycled moisture originates from transpiration rather than evaporation, which produces water vapour with lower  $\delta^{18}$ O values. These findings had important implications for the interpretation of carbonate isotope records in speleothems, since they could be compared with local  $\delta^{18}$ O records of precipitation from previous decades. Using local meteorological data and regional  $\delta^{18}$ O values in precipitation, a model was developed that reproduced the cave drip water  $\delta^{18}$ O record obtained during 2 years of observation. According to the matching records, it was estimated that the upper 500 µm of the speleothem grew between 1984 and 2003 and accurately

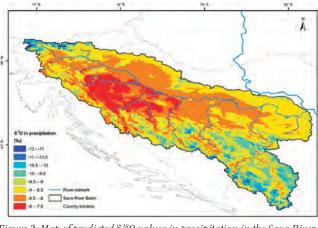


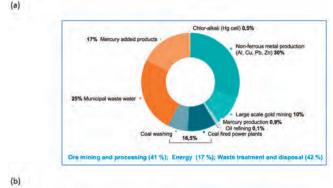
Figure 2: Map of predicted  $\delta^{18}$ O values in precipitation in the Sava River Basin.



Figure 3: Nitrate pollution sources in groundwater of Ljubljansko polje aquifer evaluated based on the stable isotope mixing model using nitrogen and oxygen in nitrate

reproduced the variability of the O isotopes in regional precipitation filtered by the aquifer. We also participated in a study of speleogenesis of a deep cave on the Nullabor Plain in Australia, based on the sulphur ( $^{34}/^{32}$ S) isotope composition of gypsum formations in the cave. High (positive)  $\delta^{34}$ S values of both surface and cave gypsum argue against gypsum genesis via microbial chemoautotrophy, or sulphuric acid speleogenesis, and are rather attributed to the atmospheric (sea spray) origin of sulfur.

We have also investigated the occurrence of Cr(VI) in the sediments of the Sava River from industrially impacted sites. Cr(VI) was mostly not detected, or its concentrations were very low, and did not exceed 0.005 mg Cr(VI)/kg. With partners from the Institute for Biological Research Siniša Stankovič (IBISS) from Belgrade, Serbia the contamination of the riparian soil was investigated along the Sava River. Measures should be taken to prevent contamination of the riparian soil by agricultural and industrial activities. Further, we studied the behaviour of selected, potentially toxic elements (PTE) in the water, sediments and fish from the Evrotas River, Greece. Perturbation of sediments during flash flood events partially remobilises contaminants accumulated in sediments into overlying waters. Consequently, PTE in water samples, associated with particulate matter were significantly increased in water samples under high



Birth cohort studies 23,374 mother-child pairs 47,699 biomarker measurements

Figure 4: Within the UNEP/AMAP report "Global mercury assessments" as a technical background document for the implemntation of the global mercury convention, the Minmata Convention, the department has made a significant contribution in two segments: (a) the calculation of global anthropogenig releases of Hg into aquatic environments.; the figures in the graph show data without input from artisinal small-scale gold mines representing an additional 600 tonnes a year (ASGM) (b) a report on mercury exposure globally, indicating a lack of data, and points to the exposure of the most vulnerable population in an early age of life.

water discharges, while under drought conditions, the dissolved contents of PTE in river water were significantly higher than during high water discharges. Similar behaviour of PTE was also observed in the Sava River. In sediments, elevated Cr and Ni concentrations, similar to those found in the Sava River, were from geogenic origin, while in the Sava the sediments derived from anthropogenic activities. In Evrotas fish, concentrations of PTE were low. In collaboration with researchers from Spanish National Research Council from Barcelona, Spain, we examined the behaviour of organic nanomaterials in the Sava River. Concentrations of fullerene C60 determined in the Sava River water were appreciably higher during drought conditions than under high water levels. These data indicate a higher environmental burden of dissolved and nano-sized contaminants under drought conditions. With the Spanish group, the occurrence of persistent organic pollutants in the Sava fish was also studied. The results indicated on elevated concentrations of dioxin-like substances in predator fish from the lower Sava stretch. Together with researchers from the Rudjer Bošković Institute, Zagreb, Croatia, we have performed sedimentological and geochemical characterizations of river suspended particulate matter sampled by time-integrated mass flux sampler (TIMS) in the Sava River (Croatia), while with researchers from Tubingen University, Germany, particle bound pollutants related to suspended sediment were evaluated in the GLOBAQUA river basins.

Condition indices, stable isotops and (semi)metals in samples of *Mytilus galloprovincialis* mussels were determined to evaluate the environmental status of the Adriatic Sea in the region of Istria. Special attention was paid to arsenic speciation, which was together with selenium and mercury also studied in the muscle and liver tissues of thunas from East Pacific (*Thunnus albacores* and *Katsuwonus pelamis*). The effects of arsenite and arsenate uptake to xerohalophyte bush *Atriplex atacamensis* was studied and the suitability of this desert plant for phytoremediation of polluted soil was evaluated.

In the framework of the implementation of the Global Minamata Convention, we actively participated in the preparation of recommendations for the implementation of survellance programmes in order to monitor the effectiveness of its implementation at the global level. We prepared the

GMA report (Figure 4a and b)) and the implementation of the WHO and UNEP Pilot Project on the preparation and implementation of human monitoring, with which we can monitor the exposure and negative effects on health. We have also made recommendations at the national level.

Radon (Rn) in ambient air was used as an indicator to study the vertical mixing of air in the lower atmosphere. In Ljubljana and Ajdovščina, the activity concentration of radon in air has been monitored continuously (1.5 m above ground, once per hour) and the meteorological parameters were obtained by the Environmental Agency of the Republic of Slovenia. Time series of Rn activity concentration and meteorological data, were analysed in order to identify geophysical parameters causing deviations of radon levels from their seasonal averages, and to use radon as a tracer of vertical air mixing. Based on the time series of radon activity concentration for Ljubljana, we built a model for the identification of persistent temperature inversion events in winter and tested it on particulate matter in the air (PM10). The time series of the radon concentration for Ljubljana and Ajdovščina were used to determine the stability classes of the atmosphere in summer, applying the so-called ,radon-based stability' method. The method is selective and gives very good results.

Within several radon-prone areas in Slovenia, we focused on the carbonate rocks and tectonic fault, where the dynamics of indoor radon in several individual houses was investigated for a year. In the first house, beside carbonate rocks beneath the house, the proximity of a well was responsible for a high concentrations of radon. In the living room in the ground floor, the average concentration of radon in the cold season reached more than 11 k Bq m<sup>3</sup>. In two houses with elevated radon concentrations of indoor radon and, hence, on the received effective doses of the occupants. The effective dose was calculated on the basis of all-day (0-24h) and night (22-6h) radon concentrations. The second approach gave on average by a factor of 1.05 higher dose than the first one. The effective dose based on night-time concentration (22-6h) was on average 4.9 times higher in the winter than in the summer.

#### Microbial system ecology

Using methods of systemic microbiology we conducted research of human oral microbiology. We compared the microbiome of healthy volunteers with patients who developed paradontal disease. From healthy volunteers

we successfully isolated microorganisms belonging to the genus *Bacillus*, which according to our analysis enable the healthy functioning of the oral community and prevent the spread of pathogenic microbes. Their antimicrobial activity against oral pathogens such as *Aggregatibacter actinomycetemcomitans* was investigated. Based on our investigation and in cooperation with experts from the Faculty of Pharmacy, University of Ljubljana, we have developed a special delivery system that enables the effective introduction of these Bacillus probiotic bacteria into gum pockets in people with progressive paradontal disease.

In addition, in cooperation with the University of Tomsk, we developed a method for testing materials for the purpose of controlling the bacterial growth on bone implants. In doing so, we developed a new method for the

contact testing of coatings. Based on our research we have shown that a properly surface-treated hydroxyapatite can be very unfavorable for the attachment of bacteria and biofilm spread.

With researchers from the Medical Faculty and the Faculty of Mechanical Engineering, University of Maribor, we have developed a system for the delivery of probiotic bacteria of the species *Staphylococcus epidermidis* for prophylaxis and treatment of diabetic foot ulcers. The probiotic bacteria which we used in the study were newly isolated from the skin of healthy individuals in our laboratory.

In the department, we also dealt with the tremendous health problem of an increasing number of antibiotic-resistant bacteria. As the first in the

world, we have shown the effects of the structural properties of DNA on the interaction of genes in bacteria. By using the physical properties of DNA in non-coding regions, we predicted a section of DNA that can be transferred to other bacteria and the repertoire of new hosts of these genes. This procedure enables the selection of appropriate combinations of antibiotics that reduce the transmission of resistance between bacteria.

#### Environment and health

Our main task is to support and interlink environment, health, and food-related studies at all steps, from planning to data interpretation. Food is a source of energy, but also the main transport route of contaminants and pathogens and as such a conspicuous way to prevent diseases.

In the frame of the national CRP project Exposure of children and adolescents to selected chemicals through their habitat environment, coordinated by our department, recruitment and sampling campaigns were conducted in 2018. Sampling of children aged 6-9 years and adolescents 12-15 years was carried out at selected schools in the area of Prekmurje, following a protocol that was prepared in 2017. We collected samples of 250 children. The list

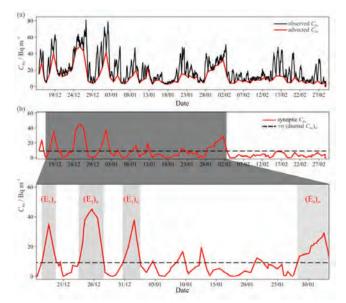


Figure 5: (a) Hourly mean observed radon concentrations with the advected contribution indicated, and (b) isolated synoptic timescale radon concentration in winter with the standard deviation of the diurnal contribution indicated. Four 'persistent temperature inversion' events (Ei)W detected by the Radon-Based Stability Method are shown in the shaded area and enlarged in the breakout panel beneath.

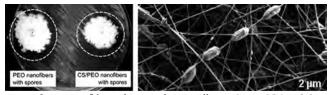


Figure 6: Activity of the probiotic isolate Bacillus sp. Strain 25.2.M (A) incorporated in nanofibers (B) against pathogenic bacterial cells A. actinomycetemcomitans

of chemicals to be determined in the collected samples includes trace elements, phthalates and DINCHs, bisphenols, flame retardants, PAH, and pesticides. The selection of chemicals is harmonised with the European Human Biomonitoring Programme (HBM4EU, Horizon 2020), which set these chemicals on a priority list in relation to health. In the HBM4EU project, we cooperated in several work packages in 2018. The main activities as cadmium group leader were: a) development of a methodological protocol for the processing of existing cadmium data, b) identification of existing studies that are suitable for inclusion in processing, c) participation in the preparation of a plan for a Cd risk-assessment study, d) preparation of a document for identifying potential biomarkers of the effect on the basis of known toxicokinetic and epidemiological data for Cd. We have successfully organised and executed the First Interlaboratory Comparison Investigations (ICI) on Cr in whole blood, serum and urine. In addition, we participated in the preparation of two training courses in the framework of HBM4EU, the first being hosted at O2 (Reactor Centre).

We have prepared a national HBM program for the period 2018-2022, which has been approved by the Chemical Office of the Ministry of Health of the Republic of Slovenia. The programme includes the above-mentioned priority groups of chemicals, and will be implemented in several areas all over Slovenia according to the protocol established in the CRP project and piloted in the area of Prekmurje.

We have started with the implementation of the ARRS project - Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population (NEURODYS), in which we continue with the use of available data from previous and current studies (PHIME, CROME, HEALS) and with the additional chemical, biochemical and molecular analyses to fill the existing data gaps. The main objective of the project is to establish a link between exposure to chemicals from the environment, human (epi)genome and neuropsychological performance, taking into account the microbiome. Advanced methods of machine learning and bioinformatics are used in collaboration with the Department of Knowledge Technologies, E8, and the Department of Molecular and Biomedical Sciences, B2. In connection with epigenetics, we attended a training at the Karolinska Institute in Sweden in 2018 on the pyrosequencing and the use of bioinformatics tools for the processing of epigenetic data. Within this project, a new study population of mother/child pairs is planned. An agreement was arranged with the General Hospital Celje to recruit mothers through gynaecological clinics and to ensure the collection of biological materials needed for the study at the Celje Maternity Hospital.

Within the NEURODYS project, we have set up sequencing methods for DNA and RNA molecules using the third generation of sequencers. We have established protocols for the analysis of human microbiome in samples of faeces of adult volunteers and infants. For the analysis of microbimes we prepared a special DNA isolation method and established all bioinformatics methods: methods for determining the quality of sequences, filtration procedures of the highest-quality sequences, sequencing based on BLAST algorithms, statistical and bioinformatic analysis of ratios of representatives of communities, alpha, beta and gamma diversities. We also introduced bioinformatic methods of predicting the function of microorganisms based on the sequence of 16S rRNA genes, which enables us to evaluate the metabolic potential of a particular microbial group.

In the field of human biomonitoring, we extended our method for analyzing BPA in urine by including the two bisphenols: BPF and BPS. It also included using our newly acquired positive-pressure extraction manifold designed for biological samples. This makes the analytical method more reproducible and less time consuming (greater sample through-put) compared to a solid-phase extraction vacuum manifold. We have now revalidated the new method. In addition to this, we have begun developing a non-target workflow also for urine. In the meantime, we have determined the population groups and the number of samples that will be analyzed within Work Package 16 of the HBM4EU project.

In parallel to analytical methods, we have also been active in the area of toxicity research. We have continued exploring ecotoxicity (in collaboration of National Institute of Biology and Faculty of Health Sciences, University of Ljubljana) and estrogenicity (Department of Molecular and Biomedical Sciences, JSI) of parent compounds (bisphenols), their mixtures and influents and effluent from pilot-scale bioreactors and photoreactors. The results indicate that despite bisphenols sharing a common structural backbone, i.e., bridged phenols, they vary greatly in their physicochemical properties (e.g., Kow) and also in their ecotoxic and estrogenic potential. Besides bisphenols, we also investigated the effects of cytostatic residues and finalised a major study in collaboration with the University of Campania, Italy, on acute and chronic ecotoxicity of the cytostatics: cyclophosphamide and ifosfamide residues in UV-treated samples showing how complex are the effects of mixtures of environmental contaminants.

In July 2018 we prepared the training on mercury determination in human and environmental samples for participants from South America; and in November 2018 we organised a training course on elemental speciation in human and environmental samples for a group from Saudi Arabia.

For the clinical and biomedical research of arsenic trioxide as a target drug for acute promyelocytic leukaemia (APL) we followed the arsenic metabolites and the selenium status during the treatment of new patients, while the wider investigation of selected gene polymorphisms (SNPs of AS3MT, SELENOP, GPX, INMT, ALAD, etc.) was

also started in available archive samples of patients included in the As study since 2004. The same polymorphisms began to be followed for the general population (from epidemiological studies) to obtain an estimation of national genotypes frequencies for selected genes. To get a better insight into As-Se interactions we optimised the method for triselenonium ion determination in urine.

In biomedical research in collaboration with the Group for Nano-Bio Science (National Food Institute, Technical University of Denmark, Denmark) and the Swiss Federal Laboratories for Materials Science and Technology (Empa, Switzerland) we studied the translocation and accumulation of silver nanoparticles (AgNPs) in the human *ex* 

*vivo* placenta perfusion model by SP-ICP-MS (Figure 7). The results revealed that AgNPs and ionic Ag were detected in the fetal circulation in low, but not negligible, amounts. Perfusion with ionic Ag size in the fetal circulation revealed the formation of Ag-containing NPs in an amount and with their size comparable to perfusion experiments with engineered AgNPs. Our study highlights that the uptake of Ag ions and/or the dissolution of AgNPs in the tissue followed by re-precipitation in the fetal circulation needs to be considered as an important pathway in studies of AgNP translocation across biological barriers.

Analytical data was provided to the Department for Nanostructured Materials from the JSI, which produced an innovative, theranostic material based on FePt/SiO<sub>2</sub>/Au hybrid NPs for photo-thermal therapy and magnetic resonance imaging. It was confirmed that the hybrid FePt/SiO<sub>2</sub>/Au NPs were not only efficient but also highly selective photo-thermal agents.

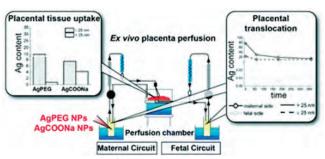


Figure 7: Translocation of silver nanoparticles in the ex-vivo human placenta perfusion model characterized by SP-ICP-MS

Furthermore, the improvement in the contrast and the easier distinction between the healthy and the cancerous tissues were clearly demonstrated with *in-vitro* MRI experiments, proving that hybrid NPs have an excellent potential to be used as contrast agents.

Within an international research team, 3D tissues model from Parkinson's disease-specific neurons derived from induced pluripotent stem cells carrying the LRRK2-G2019S mutation was developed. Imaging data show decreased dopaminergic differentiation and branching complexity, altered mitochondrial morphology, and increased cell death in LRRK2-G2019S neurons. A holistic analysis of all the studied features shows that the genetic background of the PD patients was the strongest contribution to the phenotypes and support the use of advanced *in vitro* models for future patient stratification and personalized drug development. Preclinical investigations were conducted together with the Institute of Oncology, Ljubljana on the speciation of Pt-based chemotherapeutics and their application in combined therapis, while a computer dual-porosity model was developed in the group led by a partner from the Faculty of Electrical Engineering, Ljubljana, which is a promising tool for minimizing number of experiments required in the laboratory and in the planning of modern, targeted, cancer treatments at a clinical level.

#### Environmental technologies

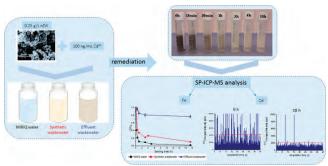
In cooperation with Limnos d.o.o., the Biotechnical Faculty and the Slovenian Forestry Institute, we want to develop new technology for sludge treatment. Thus, the influence of various treatments on the process of mineralization of sludge on sludge drying reed beds (SDRB) was studied. First measurements of the isotopic composition of respired air from the sludge indicate that on passively aerated and actively aerated observations the microbial production is higher. This indicates that sludge decomposition in those observations was higher compared to the control and can be successfully used in sludge-treatment technology.

In the field natural resources management, we continued the geochemical and hydrological investigation of coal seams in the Velenje basin, where the chemical composition, As speciation and authigenic mineralization of low-rank coal were analysed. As the concentration was comparable to other coal samples from Slovenia, however, the fraction of organoarsenic compounds in the Velenje coal was significantly higher. The mineral occurrence in the coal is important since authigenic minerals can reduce the coal's permeability, which can facilitate gas outbursts and inhibit gas extraction. Six types of calcite mineralization in a fine lignite gelified matrix were recognized, which precipitated in different conditions in a wide range of temperature (5.7–45°C), as calculated from the carbonate C and O isotope composition.

In the framework of the study of biomonitors of anthropogenic pollution in aquatic environments, we analysed the environmental status of the NE Adriatic Sea in the Istria region based on the mussel (*Mytilus galloprovincialis*) condition indices, stable isotopes of N and the concentration of metalloids. A similar study was conducted in the area of National Park Kornati in Central Adriatic, where C and N isotope compositions in a banded dye murex (*Hexaplex trunculus*) were used to identify the appropriate environmental control areas unaffected by anthropogenic pollution.

Within the EU project RusaLCA in collaboration with researchers from the Slovenian National Building Institute (ZAG), we have proved that nanoscale zero-valent iron particles (nZVI) efficiently remove pollutants and bacteria

from the effluent water from a small biological wastewater-treatment plant. However, after their use, nZVI may persit dispersed in the remediated water, representing potential nano-threats. The behaviour of nZVI and their interactions with Cd<sup>2+</sup> after remediation with different Fe loads and in different water matrices was therefore studied. For this purpose, a novel method using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) was optimized for sensitive and interference-free measurement of nZVI in environmental water matrices. The results showed nZVI sedimentation and aggregation strongly depend on water matrix. After 7 days of settling negligible concentrations of nZVI were found in the effluent wastewater, which could confirm that the use of nZVI for water remediation is safe regarding the potential environmental nano-threat (Figure 8).



*Figure 8: Investigation of the behaviour of nZVI and their interactions with Cd2+ in wastewater by single particle ICP-MS* 

In collaboration with researchers from ZAG we have obtained an EU patent: Process for obtaining health - and environment acceptable construction materials from the soil containing water soluble compounds of heavy metals: European patent specification EP 3131688 (B1), 2018-01-24. Munich: European Patent Office, 2018, and the Slovenian patent: Remediation device and the procedure for the remediation of water from small biological wastewater treatment plants: Patent SI 25327 (A), 2018-06-29.

Within the Applause project, we prepared a genetic library containing more than 10,000 isolates and clones, among which we investigated the activity of degradation of starch, inulin, cellulose and lignin. These substances are important raw materials for biotechnological conversion into useful compounds such as bioplastics from polyhydroxy alkanoates and vanillin from ferulic acid. The latter is released during the degradation of the lignin polymer. Since conventional microbial catabolism only allows

the degradation of polymers and not the modification of monomer units, the method of precise spatial positioning of different types of microbial cells in the form of aggregates has been developed within the project. For this purpose we made a prototype of aggregates of various Lac + Lac - cells of the Lactococcus lactis bacteria, which were successfully coupled to each other to breakdown lactose. In contrast, if the cells were separated the release of galactose and

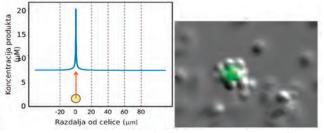


Figure 9: Bacterial cells can transfer from one cell to another different sort of chemicals, but only in the concentration gradients at a distance of a few micrometres. Because of that we developed a method that enables multicellular catalytic processes that involve different sorts of cells.

glucose from lactose was not observed (Figure 9). Analyses of aggregates and measurements of lactose degradation were carried out in cooperation with Vrije Universitat Amsterdam. This similar approach was also made in the combination of two different cell types where we aggregated the cells capable of conversion of nitrite to nitrate with Nitrobacter winogradskyi and from nitrate to gas nitrogen with the help of Pseudomonas putida.

This kind of process enables us to use a top-down approach of the specific controlled aggregation of cells, which makes it easy to upscale to the larger industrial processes of the preparation of such biocatalytic cores.

We started the cooperation with the company VO-KA and the Geological Institute of Slovenia to prepare a plan of procedures for the remediation of the soil contaminated with de-ethylatrazine in the area of the Ljubljansko barje. This study will lead to the implementation of remedial measures.

#### Environmental management, environmental impact assessment and risk assessment

In a framework of the H2020 ICARUS project (ICARUS stands for Integrated Climate forcing and Air pollution Reduction in Urban Systems) measures and polices related to air-quality improvement and the health protection of the citizens in participating cities were developed. The EU H2020 project SciShops - Enhancing the Responsible and Sustainable Expansion of the Science Shops Ecosystem in Europe was a background for establishing the first science shop in Slovenia, named Cthe entre for participatory research at JSI (Figure 10). A meeting of MODARIA II WG1 participants (MODARIA stands for Modelling and Data for Radiological Impact Assessments) was organised at the IJS in May 2018.

Based on the 5-year research within the GLOBAQUA project, regarding the Sava River, several recommendations were launched to National Environmental Agencies, International Sava River Basin Commission, and to the National Institutions for Public Health. Due to the very high Hg, MeHg and dioxins concentrations found in big and predator fish in the lower Sava stretch, which greatly exceeded (up to five times) the maximum allowable values recommended for safe consumption, eating of these fish in the lower Sava stretch should be restricted to a minimum. Measures should also be be taken to reduce the input of nutrients into the water of the lower Sava stretch.



Figure 10: Logo of the Centre for participative research at JSI

#### Environmental monitoring

The monitoring of organotin compounds in sea and surface waters was performed in collaboration with the Slovenian Environmental Agency (ARSO), while in collaboration with the Environmental Agency from Croatia, monitoring of organotin compounds and polybrominated diphenyl ethers in surface and sea water continued in 2018.

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 the Krško Nuclear Power Plant (NPP), with a determination of strontium and tritium in environmental samples, as well as tritium and radiocarbon in gas effluents from the NPP. With analyses of strontium and tritium, we also participated in the monitoring of radioactivity in the drinking water in Slovenia, as well as in the monitoring of the living environment in Slovenia. The methods used for the determination of strontium, tritium and radiocarbon for the monitoring purposes are accredited by the Slovenian accreditation body (SA LP-090).

We continued with the monitoring of the isotope composition of precipitation at 8 locations in Slovenia in the frame of the Slovenian Network of Isotopes in Precipitation (SLONIP). Since 2016, we also cooperated in the Hungarian-Slovenian project "Spatial distribution of water isotopes in precipitation in Europe with special focus on the transect from the Adriatic Coast to the Pannonian Plain". In 2018 the first geostatistical treatment of collected isotope data via GIS-supported spatial modeling tools was performed and the first regional isoscapes of the isotopic composition of precipitation across the Adriatic Coast-Pannonian Plain transect were prepared.

For the Municipality of Celje, a short applied research of radon monitoring in buildings prior to their energy renovation was conducted in the summer; radon in the indoor air was found to be mainly entering the building through the sub-floor shafts.

#### Food research and activities of the ERA Chair ISO-FOOD

The ISO-FOOD ERA Chair for isotope techniques in food safety, quality and traceability was established in 2014. In collaboration with researchers from IPREM (Pau, France) and in a framework of the MASSTWIN project, we have examined the potential of the Sr isotope composition and multi-elemental analysis for the origin discrimination of world famous brands of European dry-cured hams. With the help of statistical tools we were able to discriminate the differences between different hams. One ham in particular stood out, since in its production salt from the local brine mine is used. Its speciality was also confirmed with the <sup>87</sup>Sr/<sup>86</sup>Sr isotope ratio.

New methods were developed in food authenticity and traceability including: (i) development, optimization and validation of new GC-FID and GC-C-IRMS methods for the determination of fatty acids without derivatization; (ii) the development of the method for determining milk dilution with water using a stable isotope composition of oxygen in lactose as an internal reference; and (iii) developing the stable isotope composition of Sr for geographical origin discrimination. The Sr stable isotope analyses were performed in milk casein samples from different geographical locations in Slovenia.

In the smart specialization program "Food for Future", we studied the authenticity of raw materials such as natural flavourings in collaboration with Frutarom Etol. A dynamic headspace solid-phase micro-extraction (HS-SPME) methodology used with gas chromatography-mass spectrometry (GC-MS) and gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS) analysis was developed for compound identification and stable isotope analysis. The method was further tested on other types of fruit distillates and powdery aromas of various flavours, such as lemon, chocolate, vanilla, coconut. A database of  $\delta^{13}$ C values of apple aroma compounds with respect to their origin (synthetic and natural) was established, based on which an assessment of the authenticity of commercially available aroma compounds was performed. The sensitivity of the method was evaluated through a simple isotope mass-balance calculation. It was found that falsification identification is possible for most aromatic substances when the amount of added synthetic compound is in tens of percent.

The data of aromatic profiles using HS-SPME with GC-MSD and  $\delta^{13}$ C values obtained by GC-C-IRMS methods will also form the database of natural truffle samples to verify the authenticity of the truffle aroma in products on the market. Currently, the database consists of over 200 authentic samples of various types of white and black truffles. This work is part of the ongoing REALMed project (Pursuing authenticity and valorisation of Mediterranean traditional products) financed within the ArimNet EU scheme.

The preliminary expert task of checking the origin of selected fruits (strawberries, cherries, apples) and vegetables (garlic) using stable isotopes of light elements and elemental composition in combination with multivariate statistical methods was performed for the Administration of the Republic of Slovenia for Food Safety, Veterinary and Plant Protection. The models built using authentic fruit and vegetable samples provide a good basis for discriminating between authentic samples and those on the market with a certain degree of reliability and can help to establish an appropriate traceability system.

New research was conducted on *Spirullina* microalgae food supplements, currently available on the Slovenian market to identify their quality and safety. An experiment with the lactic acid fermentation of fresh *Spirulina* 

to potentially increase the nutritional and functional value of microalgal biomass and to easily extract bioactive components was conducted in cooperation with the Biotechnical Faculty, University of Ljubljana. The difference in proteome in yeast cells before and after fermentation was evaluated on Q-Exactive HF Orbitrap instrument at Maastricht University, Netherlands.

Within the ERAChair ISO-FOOD (2014-2019) we have continued researching the retention-sweetness relationships of a variety of artificial sweeteners and studying variations in phytoestrogen content between organically and conventionally produced beer and hops. In the latter study, an LC-MS/MS method for the analysis of three selected prenylflavonoids in hops and beer was developed and validated. We then applied this method to the analysis of a series of commercially available hops and beer produced from the sampled hops (Slovenian Institute of Hop Research and Brewing, Žalec). Samples included matched pairs of organically and conventionally produced varieties of hops from four producing countries. We found no significant difference between the content of the selected phytoestrogens, neither in hops, nor in beer. In addition, we found no significant influence of the production year within a region. In parallel, we developed a GC-MS/MS method for determining the THC content in hemp preparations intended as supplements. We have also started studying the migration of compounds from food contact material (FCM), focusing on the bisphenol migration from FCMs and the formation of their transformation products formed during various conditions in different materials (plastic bottles, reusable plastic bottles, cans, etc.) and matrices (food/ drinks and food simulants). The preliminary experiments have already been evaluated and set grounds for a detailed experimental set up, where non-target analysis will be performed in collaboration with the University of Antwerp.

Finally, in collaboration with the Faculty of Chemistry and Chemical Engineering, University of Ljubljana, we developed an analytical method for the determination of five neonicotinoid pesticides in honey using two different extraction techniques (SPE and QuEChERS) and LC-MS/MS. A validated method was applied to the analysis of 51 honey samples collected from across Slovenia in the period 2014–2016. The results revealed a low contamination of acetamiprid and thiacloprid, indicating the continuous exposure of honeybees to some neonicotinoid contamination and the threat it poses to the honeybees. In continuation, we started developing an analytical method for the determination of these compounds in a variety of propolis samples and pesticide residue determination in bees. The latter was carried out as a secondment at INIA, Madrid within the MASSTWIN project.

#### Infrastructural Centre for Mass Spectrometry (CMS)

The infrastructural Centre for Mass Spectrometry is involved in research and analytical measurements within various research programs and projects in the fields of environmental chemistry, chemistry for sustainable development, organic synthetic and pharmaceutical chemistry, biochemistry, medicine and other natural sciences fields, whose holders are research groups at the JSI, the National Institute of Chemistry, the National Institute of Biology, the University of Ljubljana, Maribor and Nova Gorica, Centers of Excellence, the partners from the Slovenian industry, etc.

With the high-resolution tandem mass spectrometer Q-Tof, coupled to the chromatographic methods LC-MS and GC-MS, the structure of various organic compounds, organometallic complexes, biopolymers, pollutants and other chemicals were determined. We studied new synthetized organic compounds, active substances, proteins, lipids and similar organic and biomolecules, ceramic materials, food supplements and food additives, monitoring pollutants in the environment, food and other matrices.

We have investigated and published in the Journal of Analytical Methods and Chemistry, the antidiabetic effect of fomentariol, a natural active substance isolated from the mushroom Fomes fomentarius. In cooperation with the University of Maribor and the public company Vo-ka d.o.o. we published in the Water research magazine two studies on the pollution of the Ljubljana groundwater with benzotriazoles and their transformation products. With GC-MS measurements we monitored the concentration levels, pathways of penetration and degradation products of benzotriazoles in water at different depths of wells in the urban area. HRMS measurements with LC-MS were also used to characterize aflatoxin in foods, where plasma, laser and UV light are used for disinfection, where lower-weight molecular and metabolic products of aflatoxin were formed. The model compounds hexandiol and adipic acid were used for the efficiency testing of the effluent treatment with photo- and electro-catalytic processes in a pilot reactor. Their concentration was monitored by LC-MS measurements at different times and energies of irradiation. In all of the above studies, an accurate mass spectrometric measurement for the identification of organic compounds, not target products and their degradation products, was used, which allowed the characterization of compounds and determined their impact on human health and the environment. A similar health impact was recognized in the quantitative LC-MS analysis of cannabinoids, in particular psychoactive THC and therapeutic CBD and impurities, in various medical hemp products for treating children with epilepsy at the Pediatric Hospital in Ljubljana.

#### Ecological Laboratory with a Mobile Unit

The Department of Environmental Science also operates a mobile chemical laboratory of Ecological Laboratory with a Mobile Unit (ELMU), which is also involved in the Civil Protection and Rescue System in Slovenia for intervention in the ecological accidents with hazardous substances and materials. In 2018, the chemical mobile laboratory of ELME intervened in the field eight times due to environmental pollution, mainly due to the spills of hazardous substances into the water streams and indirectly threatened sources of drinking water and irregular waste disposal. Within the framework of the project Modernization of mobile chemical laboratory ELME, we acquired in 2018 a portable mass spectrometer GC-MS Torion T-9 and portable aerosol spectrometer. With these instruments we will improve and update the procedures for the detection and characterization of hazardous substances in the air, waters and soils in the case of accidents involving hazardous substances, pollution and endangering human health. The members of the mobile chemical laboratory were trained, especially in regular ELME exercises, to work with new equipment and improved the knowledge, procedures and analytical methods of the mobile ecological laboratory for the determination of hazardous substances in the environment

### Some outstanding achievements in the past year

- 1. We successfully passed the external audit to obtain the accreditation certificate for determining the isotopic carbon composition in ethanol and the isotopic composition of oxygen in water in food samples.
- 2. We developed a method to verify the authenticity of key aroma compounds
- 3. We developed a steady- and transient-state hydrological model for the determination of interactions between surface and groundwater in the Ljubljansko polje aquifer and used it for future predictions of water scarcity
- 4. In collaboration with researchers from the Technical University of Denmark and the Swiss Federal Laboratories for Materials Science and Technology we demonstrated that SP-ICP-MS is a promising technique to study the translocation and accumulation of AgNPs in placental tissue samples, which could help to identify strategies towards the prevention of the placental transfer of nanomaterials.
- 5. The entry of 4 CMCs in the BIPM KCDB database in July 2018 for the category "Sediments, soils, ores and particulates" for As, Cd, Fe and Mn
- 6. In cooperation with the Faculty of Pharmacy, University of Ljubljana we developed a delivery system on the basis of nanofibers to deliver probotic Bacillus bacteria for the treatment of paradontal disease
- 7. We developed a method for preparing bicatalytic cores using an aggregation approach and we measured their activities in cooperation with researchers from Vrije Universitat Amsterdam
- 8. We won an OECD prize for innovation: the preparation of the biocatalytic cores for the transformation of the biomass of alien plant invasive species

### Some outstanding publications in the past year

- J. Vidmar, K. Loeschner, M. Correia, E. H. Larsen, P. Manser, A. Wichser, K. Boodhia, Z. S. Al-Ahmady, J. Ruiz, D. Astruc, T. Buerki-Thurnherr. Translocation of silver nanoparticles in the ex vivo human placenta perfusion model characterized by single particle ICP-MS. *Nanoscale*, 10 (2018) 11980-11991. IF 7.233
- F. Barbone, V. Rosolen, M. Mariuz, M. Parpinel, A. Casetta, F. Sammartano, L. Ronfani, L. Vecchi Brumatti, M. Bin, L. Castriotta, F. ValentF, D.L. Little, D. Mazej, J. Snoj Tratnik, A. Miklavčič Višnjevec, K. Sofianou, Z. Špirić, M. Krsnik, J. Osredkar, D. Neubauer, J. Kodrič, S. Stropnik, I. Prpić, O. Petrović, I. Vlašić-Cicvarić, M. Horvat. Prenatal mercury exposure and child neurodevelopment outcomes at 18 months: results from the Mediterranean PHIME cohort. *Int. J. Hyg. Environ. Health*, 222 (2019) 9-21. IF 4.848
- J. Snoj Tratnik, T. Kosjek, E. Heath, D. Mazej, S. Čehić, S.P. Karakitsios, D. Sarigiannis, M. Horvat. Urinary bisphenol A in children, mothers and fathers from Slovenia: overall results and determinants of exposure. *Environ. Res.*, 168 (2019) 32-40. IF 4.732
- A. Stajnko, Z. Šlejkovec, A. France-Štiglic, A. Sešek-Briški, I. Prpić, Z. Špirić, M. Horvat, D. Mazej, I. Falnoga. Arsenic metabolites; selenium; and AS3MT, MTHFR, AQP4, AQP9, SELENOP, INMT, and MT2A polymorphisms in Croatian-Slovenian population from PHIME-CROME study. *Environ. Res.*, 170 (2019) 301–319. IF 4.732
- 5. E. Schynider, M. Štrok, Z. Kosonen, M. Skudnik, D. Mazej, Z. Jeran, L. Thöni. Lead concentrations and stable lead isotope ratios in moss in Slovenia and Switzerland. *Ecol. Indic.*, 95 (2018) 250-259. IF 3.983
- R. Jaćimović, M.A.B.C. Menezes, G. Kennedy, P. Vermaercke. Losses of Cr content in plant samples using digestion procedures with acids, *J. Radioanal. Nucl. Chem.*, 315 (2018) 731-741. IF 1.181
- C. Russo, M. Lavorgna, M. Česen, T. Kosjek, E. Heath, M. Isidori. Evaluation of acute and chronic ecotoxicity of cyclophosphamide, ifosfamide, their metabolites/transformation products and UV treated samples. *Environ. Pollut.*, 233 (2018) 356-363. IF 4.358

- 8. M. Česen, D.J. Heath, M. Krivec, J. Košmrlj, T. Kosjek, E. Heath. Seasonal and spatial variations in the occurrence, mass loadings and removal of compounds of emerging concern in the Slovene aqueous environment and environmental risk assessment. *Environ. Pollut.*, 242 (2018) 143-154. IF 4.358
- 9. M. Ocvirk, N. Ogrinc, I.J. Košir. Determination of the geographical and botanical origin of hops (Humulus lupulus L.) using stable Isotopes of C, N, and S.*J. Agric. Food Chem.*, 66 (2018) 2021-2026. IF 3.154
- N. Ogrinc, D. Kocman, N.R. Miljević, P. Vreča, J. Vrzel, P. Povinec. Distribution of H and O stable isotopes in the surface waters of the Sava River, the major tributary of the Danube River. *J. Hydrol.*, 565 (2018) 365-373. IF 3.727
- Š. Zupančič, T. Rijavec, A. Lapanje, M. Petelin, J. Kristl, P. Kocbek. Nanofibers with incorporated autochthonous bacteria as potential probiotics for local treatment of periodontal disease. *Biomacromolecules*, 19 (2018) 4299-4306. IF 5.246
- R.V. Chernozem, M. Surmeneva, B. Krause, T. Baumbach, V.P. Ignatov, O. Prymak, K. Loza, M. Epple, F. Ennen, A. Wittmar, M. Ulbricht, E. Chudinova, T. Rijavec, A. Lapanje, R. Surmenev. Functionalization of titania nanotubes with electrophoretically deposited silver and calcium phosphate nanoparticles: Structure, composition and antibacterial assay. *Mater. Sci. Eng. C.* 2018, [in press]. IF 5.080
- M. Kurečič, T. Rijavec, S. Hribernik, A. Lapanje, K. Stana-Kleinschek, U. Maver. Novel electrospun fibers with incorporated commensal bacteria for potential preventive treatment of the diabetic foot. *Nanomedicine*, 13 (2018) 1583-1594. IF 6.692
- 14. J. Zrimec, A. Lapanje. DNA structure at the plasmid origin-of-transfer indicates its potential transfer range. *Sci. Rep.*, 8 (2018) 1820-1-1820-10. IF 4.122

### Awards and Appointments

- 1. Award for the best presentation at the conference: Vrzel, J., Ludwig, R., Ogrinc, N. Understanding of groundwater and surface water as a single system in the Ljubljansko polje, Slovenia. *GLOBAQUA final conference: water river management under water scarcity and multiple stressors, 17-19 December 2018, Barcelona (Spain).*
- Best Poster Award: Award ISO-FOOD: Hamzić Gregorčič, Staša, Ogrinc, Nives, Zuliani, Tea. Optimisation of the method for Sr isolation from the matrix for reliable determination of <sup>87</sup>Sr/<sup>86</sup>Sr isotope ratio by MC-ICP-MS in milk. 10<sup>th</sup> Jožef Stefan International Postgraduate School Students' Conference and 12<sup>th</sup> Young Researchers' Day 10<sup>th</sup> and 11<sup>th</sup> May 2018, Piran, Slovenia. Ljubljana: 2018.
- Award for poster: Plestenjak, Gregor, Vodnik, Dominik, Ogrinc, Nives, Krajnc, Bor, Ferlan, Mitja, Mihelič, Rok, Eler, Klemen. Could the additional air supply enhance the decomposition processes in sludge drying reeds beds? 16th IWA International Conference on Wetland Systems for Water Pollution Control, 30 September - 4 October 2018, Valencia, Spain. Valencia: International Water Association. 2018.
- 4. **Prešeren's Award** for a Master's thesis **Jasmina Masten**, entitled: Parameters of quality of salads, tomatoes and peppers from shops. 2018
- 5. OECD Innovation Award, Aleš Lapanje: Biocatalytic Aggregates for the Conversion of Biomass Invasive Plants into Useful Products. Paris, 19-20 November, 2018

### Organization of conferences, congresses and meetings

- 1. ERA Chair ISO-FOOD for isotopic techniques in food quality, safety and traceability Mid-term review, JSI Jamova 39, 2–23 February 2018
- 2. Modaria II Working Group: 2018 Interim Meetings of MODARIA II Working Group 1 on "Assessment and Decision Making of Existing Exposure Situations for NORM and Nuclear Legacy Sites" in Working Group 3 on "Assessment and Control of Exposures to the Public and Biota for Planned Releases to the Environment", Reactor centre JSI, Ljubljana, 7–11 May 2018
- 3. 13th ISO-FOOD Executive Committee Meeting, JSI Jamova 39, 17 May 2018
- 4. Meeting within the MASSTWIN project Waters from resource to management with isotope techniques, Reactor centre JSI, Ljubljana, 21 May 2018
- 5. 1<sup>st</sup> HBM4EU Training School, Reactor centre JSI, Ljubljana, 18-22 June 2018
- 6. Mercury Analysis and Speciation Training Course, Reactor centre JSI, Ljubljana, 9-20 July 2018
- 7. IAEA MEETING and MASSTWIN Stakeholder meeting: »Food Authenticity and Traceability«, Reactor centre JSI, Ljubljana, 3–7 September 2018
- 8. E-DWD Workshop: "Workshop on the Implementation of EURATOM, Drinking Water Directive 2013/51/ EURATOM", Brussels, Belgium, 4–5 October 2018
- 9. Trace Element Speciation Training Course: Training in Speciation Analysis, Reactor centre JSI, Ljubljana, 15–26 October 2018

- 10. ArimNET REALmed 1st Annual Meeting, Reactor centre JSI, Ljubljana, 25-26 October 2018
- 11. Meeting of the Executive Board ISO-FOOD, ERA Chair, JSI Jamova 39, 6 November 2018
- 12. Meeting on the establishment of the Center for Participatory Research at the Jožef Stefan Institute, JSI Reactor Centre, Ljubljana, 29 November 2018
- IAEA Education in the framework of the project: INT7019: Supporting a Global Ocean Acidification Observing the Network for Increased Involvement of Developing States, Reaction Center JSI, Ljubljana, 10–14 December 2018

### Patents granted

- Ana Mladenovič, Primož Oprčkal, Nina Kržišnik, Radmila Milačič, Janez Ščančar, Andrijana Sever Škapin, Process for obtaining health - and environment acceptable construction materials from the soil containing water soluble compounds of heavy metals, EP3131688 (B1), European Patent Office, 24. 01. 2018.
- 2. Ana Mladenovič, Primož Oprčkal, Radmila Milačič, Janez Ščančar, Janja Vidmar, Andrijana Sever Škapin, Peter Nadrah, Alenka Mauko Pranjić, Mirko Šprinzer, Method and system for the potabilization of effluents from biological WWTPS, SI25327 (A), Urad RS za intelektualno lastnino, 29. 06. 2018.

### INTERNATIONAL PROJECTS

- 1. Analyses of Metals, TBT and DBT in Sediments, Mussels and Fish
- Prof. Janez Ščančar
- Small Services Dr. Tiaša Kanduč
- 7FF HEALS; Health and Environment-wide Associations Based on Large Population Surveys
  - Prof. Milena Horvat
  - European Commission
- 4. 7FP GLOBAQUA; Managing the Effects of Multiple Stressors on Aquatic Ecosystems Under Water Scarcity
- Prof. Radmila Milačič European Commission
- 5. 7 FP; ERA CHAIR ISO-FOOD Era Chairs for Isotope Techniques in Food Quality, Safety and Traceability
  - Prof. Milena Horvat
  - European Commission
- 6. MeTra; EMRP Traceability for Mercury Measurements Prof. Milena Horvat
- Euramet E.v. 7. EMPIR; ENVCRM - Matrix Reference Materialls for Environmental Analysis Prof. Milena Horvat
  - Euramet E.v.
- 8. COST ES1403 New and Emerging Challenges and Opportunities in Wastewater Reuse (NEREUS)
  - Prof. Ester Heath Cost Office
- 9. EMPIR; SIRS Metrology for Stable Isotope Reference Standards Prof. Nives Ogrinc
  - Euramet E.v.
- The Use of Stable Isotopes and Elemental Composition for Determination of Authenticity and Geographical Origin of Milk and Dairy Products; Accessible Technologies for the Verification of Origin of Dairy Products as an Example Control System... Prof. Nives Ogrinc
  - IAEA International Atomic Energy Agency
- Enhancing Nuclear Analytical Techniques to Meet the Needs of Forensic Sciences; Forensics with Nuclear Methods: Art and Food Forgery, Drugs in Hair Dr. Radojko Jaćimović
- IAEA International Atomic Energy Agency 12. EMPIR - MercOx; Metrology for Oxidised Mercury
  - Prof. Milena Horvat Euramet E.v.
- Characterization of ERM-BB185, Elements in Bovine Liver Dr. Radojko Jaćimović
- European Commission
- 14. Characterization Study of Certified Reference Material of ERM-BB185 by k0-INAA and ICP-MS Methods
  - Asst. Prof. Tea Zuliani
- European Commission 15. Training Fees for Mr Dalerjon Khojiboev
- Asst. Prof. Zdenka Šlejkovec Ictp - Centro Internazionale Di Fisica Teorica
- ERDF UIA; APPLAUSE Alien Plant Species From Harmful to Useful with Citizens Let Activities

Asst. Prof. Aleš Lapanje

- European Regional Development Fund (erdf) 17. Characterisation of ERM-CE101 by k0-INAA, CVAAS in ICP-MS Dr. Radojko Jaćimović
- European Commission
   ESSEM COST ES1404; A European Network for a Harmonised Monitoring of Snow for the Benefit of Climate Change Scenarios, Hydrology and Numerical Weather Prediction Dr. Polona Vreča Cost Office
- 19. Stability Study of Reference Materials ERM-CA400 and ERM-CA713 Prof. Milena Horvat
- European Commission 20. COST CA 15202; Self-healing As preventive Repair of COncrete Structures Asst. Prof. Aleš Lapanje
  - Cost Association Aisbl
- 21. Use of Isotope Techniques for the Evaluation of Water Sources for Domestic Supply in Urban Areas; Multi-isotope characterization of water resources for domestic supply in Ljubljana, Slovenia Dr. Polona Vreča
  - IAEA International Atomic Energy Agency
- Training Fee for IAEA"s Fellow Mr Ahmad Mahmoud Abujazar, (JOR7006), 26.11.2018-21.12.2018
- Asst. Prof. Marko Štrok
- IAEA International Atomic Energy Agency
- 23. Training Fees for Mr Kyrylo Korychenskyi Prof. Borut Smodiš
- Ictp Centro Internazionale Di Fisica Teorica
- H2020-IGOSP; Integrated Global Observing Systems for Persistent Pollutants Prof. Milena Horvat European Commission
- H2020 ICARUS; Integrated Climate Forcing and Air Pollution Reduction in Urban Systems
- Prof. Milena Horvat
- European Commission 26. H2020 - HBM4EU; European Human Biomonitoring Initiative
- Prof. Milena Horvat
- European Commission
- 27. H2020 SciShops.eu; Enhancing Responsible and Sustainable Expansion of the Science Shops Ecosystem in Europe
- Prof. Milena Horvat
- European Commission
   28. H2020 MEET-CINCH; A Modular European Education and Training Concept in Nuclear and RadioChemistry
  - Asst. Prof. Marko Štrok
  - European Commission
- H2020 NEUROSOME; Exploring the Neurological Exposome Prof. Milena Horvat European Commission
- Halopeen commission
   HASSTWIN; Spreading Excellence and Widening Participation in Support of Mass Spectrometry and Related Techniques in Health, Environment, and Food Analysis Prof. Milena Horvat European Commission
- Effects of Electrostatic Modifications of Bacterial Cells on their Physiology: Growth, Division, Expression

Asst. Prof. Aleš Lapanje

Slovenian Research Agency

- 32. Formation and Growing Process of the Radioactive Aerosols including Radon and Thoron Decay Products under Different Climate Conditions in Hungary and Slovenia Prof. Janja Vaupotič Slovenian Research Agency
- Geographic Sourcing of Milk and Milk Powder using Elemental and Stable Isotope Composition
  - Prof. Nives Ogrinc
  - Slovenian Research Agency
- 34. Methods for Trace Elements Preseparation and Determination in Some Minerals and Other Inorganic Substances Dr. Radojko Jaćimović
- Slovenian Research Agency
- Dynamics of Soil Air Components (Radon, Carbon Dioxide, and its Carbon Isotopes) under Semi-Natural Forest Sites
- Prof. Nives Ogrinc Slovenian Research Agency
- Sewage Sludge Recycling through Agricultural Utilization Dr. Radojko Jaćimović
- Slovenian Research Agency
- Determination of Geographical Origin of Honey by Using Multi-Element and Isotopic Analysis of Soil, Plants and Honey Asst. Prof. Tea Zuliani
- Slovenian Research Agency
- Photochemical Fate and Treatment of Pharmaceutical Contaminants in Drinking Water Asst. Prof. Tina Kosjek
- Slovenian Research Agency 39. Mass Balance of Mercury in the Mediterranean Sea Prof. Milena Horvat Slovenian Research Agency

### RESEARCH PROGRAMS

- 1. Modelling and environmental impact assessment of processes and energy technologies Prof. Borut Smodiš
- Cycling of substances in the environment, mass balances, modelling of environmental processes and risk assessment Prof. Milena Horvat

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

- 1. Modelling hydrologic response of nonhomogeneous catchments
- Prof. Sonja Lojen
- 2. Ligands bearing tzNHCs in Organometallic Chemistry and Homoheneous Catalysis: c-C and C-N Bond Formation in Water
- Prof. Ester Heath
- Closing material flows by wastewater treatment with green technologies Prof. Ester Heath
- 4. Mortality of lowland oak forests consequence of lowering underground water or climate change?
- Dr. Polona Vreča 5. Redefinition and revival of copper-free Sonogashira cross-coupling reaction
- Prof. Ester Heath6. Non-traditional isotopes as identifiers of authigenic carbonates
- Prof. Sonja Lojen 7. Nanomedicines with antibiotics and probiotics for local treatment of periodontal
- disease
- Asst. Prof. Aleš Lapanje
- Clinico-pharmacological approach to optimize the therapeutic bleomycin concentration in patients undergoing electrochemotherapy Asst. Prof. Tina Kosjek
- 9. Ionom of crop plants for safe and quality food production
- Prof. Nives Ogrinc
- 10. Bisphenol A alternatives: transfer from food contact material, fate and human exposure Prof. Ester Heath
- 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
- Stable isotopes in the study of the impact of increasing CO2 levels on C and Hg cycling in coastal waters Prof Nives Optinc
- Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS Prof. Milena Horvat
- 14. Influence of geotechnical fills from recycled materials on groundwater Prof. Radmila Milačič

- EcoFAR: Food security and climate change mitigation by means of ecological farming development - conservation tillage, bioeffectors and sustainable weed management Prof. Nives Ogrinc
- Improved treatment and monitoring of Water Framework Directive priority pollutants Prof. Ester Heath
- Illict drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments Asst. Prof. Tina Kosjek
- Potential substances of very high concern in the context of REACH regulation Dr. Davor Kontić
- 19. In situ immobilization of contaminated soil using innovative nanotechnology, for processing and use as urban soils
- Prof. Radmila Milačič 20. Exposure of children and adolescents to selected chemicals through their habitat environment
- Prof. Milena Horvat
- 21. An attempt to interpret the results of biomonitoring in conjuction with data on environmental pollution, with an emphasis on air pollution and an assessment of the potential effects of these pollutants on the health of the population Prof. Milena Horvat
- 22. Food for future F4F
  - Prof. Nives Ogrinc
- Ministry of Education, Science and Sport
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Prof. Nives Ogrinc
- Ministry of Economic Development and Technology
- Pursuing authenticity and valorization of Mediterranean traditional products Prof. Nives Ogrinc Ministry of Education, Science and Sport
- In situ immobilization of contaminated soil using innovative nanotechnology, for processing and use as urban soils
  - Prof. Radmila Milačič Ministry of the Environment and Spatial Planning
- 26. Potential substances of very high concern in the context of REACH regulation Dr. Davor Kontić
  - Ministry of Health
- Implementation of the National Humane Biomonitoring programme Prof. Milena Horvat Ministry of Health
- Exposure of children and adolescents to selected chemicals through their habitat environment
  - Prof. Milena Horvat
  - Ministry of Health
- 29. An attempt to interpret the results of biomonitoring in conjuction with data on environmental pollution, with an emphasis on air pollution and an assessment of the potential effects of these pollutants on the health of the population Prof. Milena Horvat Ministry of Health
- Services; Determination of the Isotopic Composition of Carbon in Sugar Samples Prof. Nives Ogrinc
- 31. Different Analyses
- Prof. Sonja Lojen
- 32. Small Services in the Years from 2007 to 2019
- Prof. Milena Horvat 33. Determining Elemental Content in Environmental Samples Using k0-INAA Dr. Radojko Jaćimović
- 34. Determination of Isotope Composition of Oxygen and Hydrogen in Water Dr. Polona Vreča
- Pe "Water Supply and Sewage" Podgorica 35. Determination of 87Sr/86Sr Isotopic Ratio of Olive Oils and Soil Samples Asst. Prof. Tea Zuliani
- Institute for Adriatic Crops and 36. HG Analysis in Air, Soil and Sediments and Speciation Training Course Prof. Milena Horvat
- Bccc-scrc, Technological Laboratory of 37. Mercury Analysis and Speciation Training Course Prof. Milena Horvat Saudi Food and Drug Authority
  - Saudi Food and Drug Authority

### NEW CONTRACTS

- 1. Analyses of atmospheric releases in 2018 Asst. Prof. Marko Štrok
- Nuklearna Elektrarna Krško d. o. o. 2. Off-site radiological monitoring of the Krško Nuclear Power Plant in 2018 and 2019 Asst. Prof. Marko Štrok
- Nuklearna Elektrarna Krško d. o. o.
- 3. Monitoring of radiaoactivity in drinking water in Republic of Slovenia in 2018 and 2019

Asst. Prof. Marko Štrok Ministry of Health

- 4. Testing of the geographical origin of fruits and vegetables using elemental composition and stable isotopes Prof. Nives Ogrinc
- Ministry of Agriculture, Forestry and Food
- Chemical analysis of leachates Prof. Radmila Milačič
- Zavod za Gradbeništvo Slovenije 6
- illicit drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments

### VISITORS FROM ABROAD

- Celine Gys, University of Antwerpen, Antwerpen, Belgium, 3 February-23 March 2018 1
- 2. Prof. dr. Borislav Kobiljski, European Commission, Brussels, Belgium, 22-23 February 2018
- 3. Pascal Bogner, Ludwig-Maximilians-Universität, München, Germany, 26 March-30 June 2018
- Dalerjon Khojibojev, Faculty of Metallurgy, Buston city, Tajikistan, 4.
- 30 March-18 May 2018 5. Melisa Alejandra Rodas Ceballos, Universitet de les Illes Balears, Balearic Island, Spain, 3 April-30 June 2018
- Prof. Scott Dudley Chambers, Australian Nuclear Science and Technology Organisation, Kirrawee, Australia, 13-14 April 2018
- Prof. dr. Damia Barcelo, Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Barcelona, Spain, 17-19 April 2018
- mag. Agneta Annika Runkel, Universität Bayreuth, Bayreuth, Germany, 7 May-31 December 2018
- Dr. Nelson O`Driscoll, Acadia University, New Scotland, Canada, 8 May 2018
- 10. Prof. dr. Daniele Penna, University of Florence, Florence, Italy, Dr. Tamara Marković, Croatian Geological Survey, Zagreb, Croatia, MASSTWIN Stakeholder Event "Water from resource to management with isotope techniques", Zagreb, Croatia, 21 May 2018
- 11. Maria Laimou-Geraniou, National kapodistrian University of Athens, Athens, Greece, 1-30 June 2018
- 12. Prof. dr. Waldemar Macedo, Centro de Desenvolvimento da Technologia Nuclear, Belo Horizonte, Brazil, 1-3 July 2018
- 13. Dr. Kay Knöller, Helmnoltz Centre for Environmental Research, Halle, Germany, 19-21 August 2018
- 14. Dr. Martina Furdek Turk, Ruđer Bošković Institute, Zagreb, Croatia, 1 September-31 December 2018
- 15. Prof. dr. Russell Frew (New Zealand), prof. dr. Barry Thornton (UK), prof. dr. Gabriel Bowen (USA), prof. dr. Daniel Wunderlin (Argentina), prof. dr. Gang Chen (China), dr. Noureddine Amenzou (Morocco), dr. Ryszard Wierzchnicki (Poland), dr. Ivan Podkolzin (Russia), dr. Lian Jie Bay (Singapore), dr. Champa Dewage (Sri Lanka), dr. Roksana Huque (Bangladesh), dr. Andrius Garbaras (Lithuania), dr. Federica Camin (Italy), dr. Micha Horacek (Austria), dr. Simon Kelly (IAEA, Austria), 3-7 September 2018
- 16. Dr. Ivona Krizman Matasić, Ruđer Bošković Institute, Zagreb, Croatia, 3 September-31 December 2018

Asst. Prof. Tina Kosjek

- Mariborski Vodovod d. d.
- 7. illicit drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency and vulnerability assessment of water catchments. Asst. Prof. Tina Kosjek
  - Jp Cčn Domžale-kamnik d. o. o.
- illicit drugs, alcohol and tobacco: wastewater based epidemiology, treatment efficiency 8. and vulnerability assessment of water catchments. Asst. Prof. Tina Kosiek Jp Vodovod-kanalizacija d.o.o

- 17. Dr. Maria Ângela de Barros Correia Menezes, CDTN, Belo Horizonte, Brazil, 4-13 September 2018 and 24-28 September 2018
- 18. Dr. Marta Boito, University of Parma, Novi Ligure, Italy, 6-8 September 2018
- Ines Ribeiro Coelho, National Health Institute Dr. Ricardo Jorge, Lisbon, Portugal, 19. 16-22 September 2018
- 20. Kyrylo Korychenskyi, Atoomic Energy Agency, Kyiv, Ukraine, 21 September-17 October 2018
- 21. Dr. Marco Lauteri in dr. Angela Augusti, CNR-IRET, Porano, (Italy), dr. Cristina Maguas, dr. Carla Alegria, dr. Manueal Giovanetti (Portugal), dr. Naziha Atti (Tunisia), dr. Pedro Reis (Portugal), dr. Luana Bontempo (Italy), 25-26 October 2018
- 22. Prof. dr. Petre Makreski, Institut za kemijo, Skopje, Macedonia, 5-9 November 2018
- Prof. dr. Trajče Stafilov, Institut za kemijo, Skopje, Macedonia, 5-9 November 2018
- 24. Dr. Dean Ban, Institute of Agriculture and Tourism, Poreč, Croatia, 19-20 November 2018
- 25. Dr. Smiljana Goreta Ban, Institute of Agriculture and Tourism, Poreč, Croatia,
- 19-20 November 2018 26. Dr. Marko Černe, Institute of Agriculture and Tourism, Poreč, Croatia, 19-20 November 2018
- 27. Dr. Igor Palčić, Institute of Agriculture and Tourism, Poreč, Croatia, 19-20 November 2018
- 28. Ahmad Mahmoud Abujazar, Water Authority of Jordan, Amman, Jordan, 26 November-21 December 2018
- 29. Prof. Sofie Jonsoon, University of Stockholm, Stockholm, Sweden, 27-30 November 2018
- Dr. Johannes Bieser, HZG Germany, Geesthacht, Germany, 27–30 November 2018
   Prof. Yaw Serfor-Armah, School Of Nuclear And Allied Sciences, Ghana Atomic Energy Commission, Ghana, 2-18 December 2018
- 32. Zoltán Kern, István Gábor Hatvani, Dániel Erdélvi; Institute for Geological and Geochemical Research, Research Centre for Astronomy and Earth Sciences, Hungarian Academy of Sciences, Budaörsi út 45, H-1112 Budapest, Hungary, Project meeting "Spatial distribution of water isotopes in precipitation in Europe with special focus on the transect from the Adriatic Coast to the Pannonian Plain", N1-0054, Budapest, Hungary, 5-6 December 2018
- Prof. dr. Roberto Meigikos dos Anjos (Brazil), prof. dr. Carlos Manuel Alonso Hernandez 33. (Cuba) and prof. dr. Saif Uddin (Kuwait) 10-14 December 2018
- 34. Dr. Alexandre Soares Leal, CDTN, Belo Horizonte, Brazil, 20-24 December 2018

### STAFF

- Researchers
- Prof. Ljudmila Benedik 1 Asst. Prof. Ingrid Falnoga 2.
- Dr. David John Heath
- 3. Prof. Ester Heath 4.
- Prof. Milena Horvat, Head
- 5. Dr. Radojko Jaćimović
- 6.
- Dr. David Kocman 7.
- Asst. Prof. Branko Kontić 8
- Asst. Prof. Tina Kosiek 9.
- 10. Asst. Prof. Jože Kotnik
- 11. Asst. Prof. Aleš Lapanje
- 12. Prof. Sonja Lojen
- Dr. Darja Mazej
   Prof. Radmila Milačič
- 15. Prof. Nives Ogrinc
- 16. Prof. Borut Smodiš
- 17. Prof. Janez Ščančar
- Asst. Prof. Zdenka Šlejkovec 18.
- 19 Asst. Prof. Marko Štrok
- 20. Prof. Janja Vaupotič
- 21. Dr. Polona Vreča
- 22. Asst. Prof. Tea Zuliani 23. Dr. Dušan Žigon
- Postdoctoral associates

- 24. Raghuraj Singh Chouhan, B. Sc.
- 25. Dr. Marjeta Česen, left 01.07.18
- 26. Dr. Andrija Ćirić
- 27. Dr. Jelena Golubović
- 28. Dr. Tjaša Kanduč
- 29. Dr. Davor Kontić 30. Dr. Bor Krajnc
- 31. Dr. Tomaž Rijavec
- 32. Dr. Janja Vidmar
- 33. Dr. Igor Živković Postgraduates
- 34. Tine Bizjak, B. Sc.
- 35. Jan Gačnik, B. Sc
- Joint Gačnik, B. Sc., left 01.05.18
   Tjaša Gornik, B. Sc.
- 38. Marta Jagodic, B. Sc.
- 39. Ana Kovačič, B. Sc.
- 40. Katarina Marković, B. Sc.
- Jasmina Masten, B. Sc
- 42. Dr. Majda Pavlin, left 01.08.18
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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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### PATENT APPLICATION

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- Maruša Matko, Consideration of risks connected to extreme weather events in planning of electric energy infrastructure: doctoral dissertation, Ljubljana, 2018 (mentor Branko Kontić; co-mentor Mojca Golobič).

- Primož Oprčkal, Innovative approaches for sustainable remediation of contaminated waters and soils: doctoral dissertation, Ljubljana, 2018 (mentor Janez Ščančar; co-mentor Ana Mladenovič).
- 4. Majda Pavlin, *Mass spectrometric approach for identification of mercury compounds in solid samples:* doctoral dissertation, Ljubljana, 2018 (mentor Milena Horvat).
- Sebastijan Rep, The role of <sup>18</sup>F-choline PET/CT in the diagnosis of primary hyperparathyroidism: doctoral dissertation, Ljubljana, 2018 (mentor Marko Hočevar; co-mentors Janja Vaupotič, Luka Ležaić).
- 6. Janja Vrzel, *Surface- groundwater interactions in the Ljubljansko polje aquifer system (Slovenia):* doctoral dissertation, Ljubljana, 2018 (mentor Nives Ogrinc; co-mentors Ralf Ludwig, Goran Vižintin).
- 7. Igor Živković, Seasonal changes in mercury speciation and the composition of the microbial community in the seawater in the central Adriatic sea: doctoral dissertation, Ljubljana, 2018 (mentor Milena Horvat; co-mentor Mladen Šolić).

## DEPARTMENT OF AUTOMATION, **BIOCYBERNETICS AND ROBOTICS** E-1

The research strategy within our department is unique, as it supports a variety of multi- and interdisciplinary research projects. Specifically, our research combines the fields of robotics (including intelligent control, humanoids, cognitive robotics, robot learning, and robot vision), automation, biomechanics, 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. By combining engineering and life sciences, we have been able to make significant contributions to the development of humanoid robotic systems, a planetary-habitat simulation facility, new methods for robot learning based on imitation, manikins enabling the evaluation of protective garments for industry and recreation, kinematic models of the human body that serve as a basis for the design of anthropomorphic systems, and a medical treatment for frostbite.

The department maintains the programme group "Automation, robotics and biocybernetics" in the field of Production Technologies (leader prof. dr. Igor B. Mekjavic). Members of the department Head: participate in numerous EU projects in the area of robotics and artificial intelligence, factories of the Prof. Aleš Ude future, health, and space technologies. In 2018 we coordinated two Horizon 2020 projects: ReconCell and SPEXOR. We are also active in transferring our research results to various applications through direct collaborations with industry.

Research in the area of humanoid and cognitive robotics and 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 that are capable of acquiring new knowledge through learning and to collaborate with people in their

natural environments. We also established the Laboratory for Neuromechanics and Biorobotics, which is led by prof. dr. Jan Babič. The main focus of this lab is to integrate the results of biomechanics, neurophysiology and robotics to study human motor control and develop new robot systems that can effectively assist people in their daily activities.

During the past year our research has focused on the development of cognitive robotic systems, new robot-learning methodologies, including learning for dual-arm systems and deep learning, contact modelling, robotic assistive devices, reconfigurable robotic workcells, the automation and digitalization of industrial manufacturing, studies of human physiology in extreme environments, the evaluation of protective equipment, and the development of biomedical methods.

#### Robotics

In 2018 we continued our work in the Horizon 2020 project ReconCell (A Reconfigurable robot workCell for fast set-up of automated assembly processes in SMEs, http://www.reconcell. eu/), where we have been developing new reconfiguration technologies that enable the fast setup of robotic workcells in industrial production. The proposed workcell is based on a number of novel technologies, including 1. robot programming by kinesthetic teaching, 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 the workcell elements. In the past year we successfully applied the developed approaches to five real industrial production tasks, thus demonstrating the flex-

By maintaining a critical mass of researchers in the area of robotics, automation and life sciences within one department, we have managed to foster exciting multidisciplinary projects.

Figure 1: Reconfigurable robot workcell at Automatica 2018 in Munich, Germany







In the H2020 project ReconCell we developed new methodologies for the reconfiguration of robotic workcells. The developed system was successfully applied to implement five real industrial production tasks.



Figure 2: Passive fixture reconfigured by a robot

ibility of the proposed system. The results of the ReconCell project were demonstrated at Automatica 2018, which is one of the largest industrial fairs in the world focusing on robotics.

Another important research topic in the past year was the development of new methodologies for learning and the autonomous adaptation of dual-arm assembly and service tasks. Our research in this area addresses the following issues: 1. The development of new efficient methods for the

learning and demonstration of bimanual tasks, 2. The development of new algorithms for the efficient and autonomous adaptation of bi-manual coordinated tasks to deviations that arise in an industrial task, and 3. The verification of the developed methods and algorithms on some typical industrial and domestic tasks.

Another focal point of our work in 2018 was the Horizon 2020 project AUTOWARE (http:// www.autoware-eu.org). This project focuses on the development of new digital technologies including reliable wireless networking, fog computing, reconfigurable and collaborative robotics, modular production lines, augmented virtuality, machine learning, cognitive autonomous systems, etc. These technologies are being made ready for their application in smart factories. Special attention is paid to the interoperability between them and also with legacy devices and information systems on the factory floor. Our main contribution to the project is the integration of robotics with these new digital technologies. To this end we focus on open platforms, protocols, and interfaces.

Another Horizon 2020 project in the area of robotics that started last year is CoLLaboratE – Enabling genuine human-robot collaboration for performing assembly tasks in a co-production cell (https://collaborate-project.eu). CoLLaboratE aims to revolutionize the way industrial robots learn to cooperate with human workers when performing new manufacturing tasks, with a special focus on the challenging area of assembly operations. The envisioned system for collaborative assembly will be capable of allocating human and robotic resources for executing the production plan, sharing the tasks according to the capabilities of the available actors. In this project we plan to extend our work from ReconCell – where the focus is on reconfigurable robotics cells – to modern industrial environments where humans and robots work together.

In the H2O2O project AUTOWARE advanced robot technologies are integrated into modern smart factories.

In the scope of the Horizon 2020 project SPEXOR (http://www.spexor. eu/) we implemented the control algorithm for the Spexor passive spinal orthosis with viscoelastic elements on a dedicated single board computer along with custom-made electronics for interfacing with the sensors and actuators of the exoskeleton. The control algorithm is based on a finitestate machine combined with Gaussian mixture models. We evaluated

the controller in a test setting where a group of human subjects had to perform movements that are usually found in industrial environments. To ensure safe operation of the exoskeleton, we implemented an invariance control algorithm to supervise the nominal controller and correct the control outputs if the system states are about to leave the admissible state-space region.

Finally, in the scope of the Horizon 2020 project AnDy we developed a thorough assessment method for evaluating industrial exoskeletons, and its application to a novel upper-body passive exoskeleton for arm support during overhead work. We proposed a list of evaluation criteria, which cover both objective and subjective effects of an exoskeleton, on the user and on the task being performed. We performed a laboratory study, where 12 participants performed an overhead pointing task with and without the exoskeleton, while their physical, physiological and psychological states were being monitored. We demonstrated that working with the exoskeleton reduced the shoulder's physical strain, without increasing the lower-back strain or degrading balance, and without degrading task performance. The positive effects of the exoskeleton were also visible at the global level with a significant reduction in metabolic demand. Importantly, participants' opinions about the exoskeleton were positive, in agreement with the objective measures.

#### Automation and industrial robotics

A vital mission of our department is the transfer of our research results to industrial applications. In the past year we focused on a new smart specialization program GOSTOP: Building blocks, tools and systems for factories of the future, which is coordinated by members of our department. The aim of the 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 research and development programs

joined forces to advance the concept of smart factories. We identified four 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 the 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 the predictive maintenance of each drive

system. In the second research theme, that is an adaptive robotic workcell, we develop 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 visual quality control of industrial parts. The main goal of the development of a virtual factory platform is to design and produce an intelligent, competitive and sustainable information system in a smart factory that includes the elements of robotics. This combines 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 conducts research regarding the influence of extreme environmental factors on humans as well as on the development and evaluation of technologies 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. This facility was established with the support of the European Space Agency and the European Commission (Framework 7 Programme; PlanHab project). 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 missions in the near future, novel issues connected to space habitation are very important. In particular, for 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.

We have initiated a research programme investigating the concept of physiological crosstolerance. 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, hypoxia and metabolic stress (exercise), and their respective effects on human performance, and on the characteristics of autonomic temperature regulation. To this effect we have compared exercise performance in normal temperature normoxic environments, with the performance in hypoxic and hot environments, after altitude (4000 m) and heat ( $35^{\circ}$ C) acclimation.

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* may 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.

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

We are coordinating a new program in the scope of Slovenia's smart specialization strategy GOSTOP: Building blocks, tools and systems for factories of the future.

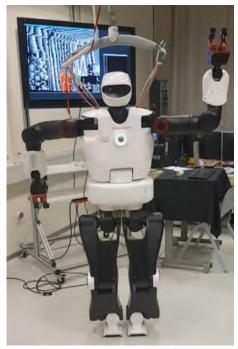


Figure 3: Humanoid robot TALOS performing dance movements



Figure 4: Exoskeleton for the prevention of back pain



Figure 5: Investigating the effect of hypoxic acclimation on exercise performance in a hot environment



Figure 6: Sweating thermal head manikin



Figure 7: Testing of compression socks

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 21<sup>st</sup> 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 the 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 well-being of 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" (www.heat-shield.eu) we are collaborating with the industrial partner Odelo d.o.o. to mitigate the detrimental

effects of heat waves on the workforce in their manufacturing plant. Within the framework of this project we have installed sensors throughout the manufacturing plant at Odelo d.o.o., and provide continuous monitoring of the conditions within the factory, particularly during heat waves. In addition, the workers provide ratings of thermal comfort, temperature sensation and fatigue at regular intervals. Preliminary analyses of the data suggest that the conditions within the factory are constant throughout the year, and that the decrease in productivity observed as a consequence of heat waves, occurs after the heat wave. This is suggestive of a cumulative effect of heat, more related to an inability to properly recover during the workers' time off work. This is one aim of our investigations in the following year. Within the framework of the Heat Shield project we are also investigating the effect of ambient temperature and humidity on thermal balance, physical performance and cognitive function, particularly with reference to the effect on the productivity of workers in manufacturing industry. In this regard, we continue to assess the available technologies and various strategies in mitigating heat stress in industrial settings, thus maintaining unhindered performance in hot environments.

With our industrial partner Kimberly-Clark (USA) we continue to 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 visual and breathing functionalities. 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 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). We are currently developing a new generation of hand manikins for our industrial partner W.L. Gore & Associates.

### Awards and Appointments

- 1. Miha Dežman: Best overall conference contribution for the ICT study programme, Piran, Slovenia, IPSS conference expert commission - 10th International Postgraduate School Students Conference, Elbow assistance exoskeleton to facilitate high level control design.
- 2. Tadej Petrič: Director's fund project for 2018, Ljubljana, Jožef Stefan Institute, project "CoBoTaT Laboratory for Advancing Collaborative Robot Behaviors in Physical Human-Robot Interaction Scenarios".
- Tadej Petrič, Leon Žlajpah: Best regular paper award, Patras, Greece, The 27th International Conference on robotics in Alpe-Adria-Danube Region, Virtual Guides for Redundant Robots Using Admittance Control for Path Tracking Tasks.

### Organization of conferences, congresses and meetings

- 1. ReconCell meeting, Ljubljana, 28. 29. 6. 2018
- 2. 7th International Conference on the Physiology and Pharmacology of Temperature Regulation (PPTR 2018), Split, Croatia, 7. 12. 10. 2018
- 3. 1st IIT JSI Workshop, Ljubljana, 22. 11. 2018
- 4. Workshop SRIP FoF "Robotics", Ljubljana, 4. 12. 2018

### INTERNATIONAL PROJECTS

#### 1. Stimulators and Parts Prof. Aleš Ude

- Kimberly-Clark Development of LCD Shutter in the Year 2018 Asst. Prof. Leon Žlajpah
- Kimberly-clark
- COST CA16116 20786; Wearable Robots for Augmentation, Assistance or Substitution of Human Motor Functions Prof. Ian Babič
- Cost Office
- ESA Individual Variation in Human Response to prolonged Bed Rest in Slovenia Bed Rest Programme Prof. Igor Mekjavić
- Esa/estec.
- H2020 HEAT-SHIELD; Integrated Inter-Sector Framework to increase the Thermal Resilience of European Workers in the Context of Global Warming Prof. Igor Mekjavić
- European Commission
- H2020 AUTOWARE; Wireless Autonomous, Reliable and Resilient Production Operation Architecture for Cognitive Manufacturing Prof. Aleš Ude
  - European Commission
- H2020 An.Dy; Advancing Anticipatory Behaviors in Dyadic Human-Robot Collaboration
  - Prof. Jan Babič
  - European Commission
- 8. H2020 CoLLaboratE: Co-production CeLL performing Human-RobotCollaborative AssEmbly
  - Asst. Prof. Bojan Nemec
  - European Commission
- H2020 ReconCell; A Reconfigurable Robot Workcell for Fast Set-up of Automated Assembly Processes in SME-s
  - Prof. Aleš Ude
  - European Commission
- H2020 SPEXOR; Spinal Exoskeletal Robot for Low Back Pain Prevention and Vocational Reintegration Prof. Jan Babič
  - European Commission
- 11. Discovery of the Optimality Criteria for Full Body Human Movements Using Inverse Reinforcement Learning
  - Prof. Jan Babič
- Slovenian Research Agency
- 12. Obstacle Avoidance as Neuroeconomical Decision Making Prof. Jan Babič
- Slovenian Research Agency 13. Stabilization of Centre of Mass to improve The Design of Light-Touch Tactile Feedback
- Robotic Canes
- 14. Prof. Jan Babič
- Slovenian Research Agency
- Establishing New Tools to facilitate New Generation Humanoid Robot Capabilities for Collaborative Human-Robot Object Manipulation

### VISITORS FROM ABROAD

- Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 10. 1.–12. 1., 17. 1.–19. 1., 24. 1.–26. 1. 2018
- 2. Lucca Tagliapietra, Italian Institute of Technology (IIT), Italy 12. 16. 2. 2018
- 3. Benjamin Schirrmeister, Ottobock SE & Co. KGaA, Germany, 12. 16. 2. 2018
- Pauline Maurice, French National Institute for computer science and applied mathematics (INRIA). France, 12, 16, 2, 2019.
- mathematics (INRIA), France, 12. 16. 2. 2018 5. prof. dr. Sami Haddadin, University in Hanover, Germany, 8. 3. 2018
- prot. dt. Saim naddadii, University in nanover, Germany, 8, 5, 2018
   Caomahan Conaghan, Athlone Institute of Technology, Ireland, 8, 13, 3, 2018
- Gasmalian Conagnan, Autoric institute of recimology, fretanti, 8. 15. 5. 2018
   Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 8. 9. 3. , 14. 15. 3., 22. -23. 3., 28. - 30. 3. 2018
- 8. dr. Tatyana Ivanovska, University of Göettingen, Germany, 3. 6. 4. 2018
- 9. Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 4. 6. 4., 11. 13. 4., 26. -27. 4. 2018

Asst. Prof. Tadej Petrič Slovenian Research Agency

 Learning Cross-Task Generalization for Model-Predictive Control: Application to Dynamic Humanoid Behaviors Asst. Prof. Andrej Gams Slovenian Research Agency

### RESEARCH PROGRAM

1. Avtomation, robotics and biocybernetics Prof. Igor Mekjavić

### R & D GRANTS AND CONTRACTS

- 1. Cardiorespiratory responses during hypoxic exercise in individuals born prematurely Asst. Prof. Tadej Debevec
- 2. Learning and autonomous adaptation of dual arm assembly and service tasks Prof. Aleš Ude
- X-ADAPT: Cross-adaptation between heat and hypoxia novel strategy for performance and work-ability enhancement in various environments Asst. Prof. Tadej Debevec
- Building blocks, tools and systems for the Factories of the Future GOSTOP Asst. Prof. Igor Kovač
- Ministry of Education, Science and Sport Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Asst. Prof. Igor Kovač
- Ministry of Economic Development and Technology 6. Strategic Research & Innovation Partnership Factories of the Fut
- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) Asst. Prof. Igor Kovač Ministru of Faceparite Davalonment and Technology
- Ministry of Economic Development and Technology 7. Testing of Thermal Resistance of Mittens
- Prof. Igor Mekjavić
- Ministry of Defence
- 8. Thermal Resistance and Dynamic Foot Test Prof. Igor Mekjavić
- Geox S.p.a.
- 9. Manufacture of Finger and Two Hands of the Manikin, and National Instruments Measuring Software
- Prof. Igor Mekjavić W. L. Gore & Associates Gmbh

### NEW CONTRACT

- Development of Integrated Torque Sensor for S-Gearbox Ultra Asst. Prof. Igor Kovač Podkrižnik d. o. o.
- dr. Maria Koskolou, National and Kapodistrian University of Athens, Greece, 11. -16. 4. 2018
- 11. Panagiotis Miliotis, National and Kapodistrian University of Athens, Greece, 11. 16. 4. 2018
- 12. Dionysios-Ermis Geladas, Greece, 11. 16. 4. 2018
- 13. Spyridoula Ntalapera, Greece, 11. 16. 4. 2018
- 14. Alexander Ketter, Logicdata, Austria, 20. 4. 2018
- 15. Manfred Spari, Logicdata, Austria, 20. 4. 2018
- 16. Frederik Hagelskjær, Syddansk Universitet, Denmark, 6. 20. 5. 2018
- 17. Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 16. 18. 5. 2018
- 18. Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 27. 29. 6. 2018
- Bo Ingemann Petersen, UAB Precizika Metal, Lithuania, 28. 29. 6. 2018
   Thomas Ronley, UAB Precizika Metal, Lithuania, 28. 29. 6. 2018



- 21. Alexander Ketter, Logicdata, Austria, 28. 29. 6. 2018
- Norbert Krüger, Syddansk Universitet, Denmark, 28. 29. 6. 2018
   Thiusius Rajeeth Savarimuthu, Syddansk Universitet, Denmark, 28. 29. 6. 2018
   Anders Prier Lindvig, Syddansk Universitet, Denmark, 28. 29. 6. 2018
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- Shahab Parizi, Blue Ocean Robotics ApS, Denmark, 28. 29. 6. 2018
   Franziska Kirstein, Blue Ocean Robotics ApS, Denmark, 28. 29. 6. 2018
- 27. Marc Priggemeyer, Rheinisch-Westfaelische Technische Hochschule Aachen, Germany, 28.-29.6.2018
- 28 Florentin Woergoetter, University of Goettingen, Germany, 28. - 29. 6. 2018
- Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 4. 5. 7., 25. -29 26. 7. 2018
- 30. Simon Reich, University of Goettingen, Germany, 22. - 27. 7. 2018
- dr. Minija Tamosiunaite, University of Goettingen, Germany, 22. 24. 7. 2018
- Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 12. 13. 9., 17. 21. 9., 26. - 27. 9. 2018
- prof. Ivan Godler, Twist Drive Technologies, Inc., Japan, 24. 27. 9. 2018
- 34. Branko Lukić, University of Belgrade, Serbia, 24. 26. 9. 2018
- 35. dr. Kosta Jovanović, University of Belgrade, Serbia, 24 .- 26. 9. 2018
- Roque Belda, HOP Ubiquitous S.L., Spain, 25. 9. 2018
- Djordje Djordjević, Ivamax, Serbia, 25. 9. 2018 37.
- Mihailo Despotović, Ivamax, Serbia, 25. 9. 2018
- 39. Zavisa Gordić, University of Belgrade, Serbia, 25. 9. 2018
- Marc Priggemeyer, Rheinisch-Westfaelische Technische Hochschule Aachen, Germany, 4025. 9. 2018

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- 22. Miha Dežman, B. Sc.
- 23. Timotej Gašpar, B. Sc.
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- 25. Jaka Jereb, B. Sc

## BIBLIOGRAPHY

### **ORIGINAL ARTICLE**

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- 2. Luka Peternel, Tadej Petrič, Jan Babič, "Robotic assembly solution by human-in-the-loop teaching method based on real-time stiffness modulation", Autonomous robots, 2018, 42, 1, 1-17.
- 3. Bojan Nemec, Nejc Likar, Andrej Gams, Aleš Ude, "Human robot cooperation with compliance adaptation along the motion trajectory", Autonomous robots, 2018, 42, 5, 1023-1035.
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- 41. prof. Atsumasa Yoshida, Osaka Prefecture University, Japan, 11. 14. 10. 2018
- Gokce Guven, Ozyegin University, Turkey, 8. 10. 14. 12. 2018
   Branko Lukić, University of Belgrade, Serbia, 2. 11. 31. 12. 2018
- 44. dr. Kosta Jovanović, University of Belgrade, Serbia, 2. 11. 31. 12. 2018
- 45. Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 9. - 11. 11., 16. - 18. 11., 24. -25. 11. 2018
- Benjamin Schirrmeister, Ottobock SE & Co. KGaA, Germany, 12. 11. 2018 46.
- Jonas Bornmann, Ottobock SE & Co. KgaA, Germany, 12. 11. 2018 47.
- Angelina Bellicha, University Pierre and Marie Curie, France, 15. 30. 11. 2018 48
- 49. dr. Arash Ajoudani, Italian Institute of Technology (IIT), Italy, 22. 11. 2018
- 50. Pietro Balatti, Italian Institute of Technology (IIT), Italy, 22. 11. 2018
- dr. Virginia Ruiz Garate, Italian Institute of Technology (IIT), Italy, 22. 11. 2018 51.
- 52. Frederik Hagelskjær, Syddansk Universitet, Denmark, 22. 11. 2018
- Marta Lorenzini, Italian Institute of Technology (IIT), Italy, 22. 11. 2018 Luka Peternel, Italian Institute of Technology (IIT), Italy, 22. 11. 2018 53. 54
- dr. Takamitsu Matsubara, NARA Institute of Science and Technology, Japan, 26. 11. 2018 55
- dr. Tsukasa Ogasawara, NARA Institute of Science and Technology, Japan, 26. 11. 2018 57.
- Masato Miyake, NARA Institute of Science and Technology, Japan, 26. 11. 2018
- Chikako Doi, NARA Institute of Science and Technology, Japan, 26. 11. 2018
- Geminias Petraitis, UAB Precizika Metal, Lithuania, 30. 11. 2018 60.
- Predrag Tadić, University of Belgrade, Serbia, 10. 12. 2018
- 61. Vladimir Šimović, Zagreb University of Applied Sciences, Croatia, 26. 30. 12. 2018

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- 26. Dr. Aljaž Kramberger, left 01.05.18
- 27. Tinkara Mlinar, B. Sc.
- 28. Rok Pahič, B. Sc.
- 29. Mihael Simonič, B. Sc.
- 30. Alexandros Sotiridis, B. Sc.
- 31. Viktor Stefanovski, left 26.09.18
- Technical officers
- 32. Mišel Cevzar, B. Sc., left 30.08.18
- 33. Rosana Černelič, B. Sc.
- 34. Tanja Dragojević, B. Sc.
- 35. Mitja Gliha, B. Sc.
- 36. Daša Gorjan, B. Sc. 37.
- Gregor Klinc, B. Sc. Tjaša Kunavar, B. Sc. 38.
- 39. Matevž Majcen Hrovat, B. Sc.
- 40. Simon Reberšek, B. Sc.
- Joshua Toby Royal, B. Sc.
   *Kaja Teraž, B. Sc., left 01.10.18*
- 43. Bogomir Vrhovec, B. Sc.
- Technical and administrative staff
- 44. Rok Goljat, B. Sc., left 01.06.18
- 45. Željka Kukec, B. Sc.
- 46. Petra Movh, B. Sc.
- 47. Primož Radanovič, B. Sc.

\* part-time JSI member

Note

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48. Danijela Zeljković Anžiček, B. Sc.

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- 15. Francesco Romano *et al.* (18 authors), "The CoDyCo project achievements and beyond: towards human aware whole-body controllers for physical human robot interaction", *IEEE Robotics and automation letters*, 2018, **3**, 1, 516-523.
- 16. Tadej Petrič, Andrej Gams, Luca Colasanto, Auke Jan Ijspeert, Aleš Ude, "Accelerated Sensorimotor Learning of compliant movement primitives", *IEEE transactions on robotics*, 2018, **34**, 6, 1636-1642.
- 17. Thiusius Rajeeth Savarimuthu *et al.* (17 authors), "Teaching a robot the semantics of assembly tasks", *IEEE transactions on systems, man, and cybernetics. Systems*, 2018, **48**, 5, 670-692.
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### INDEPENDENT COMPONENT PART OR A CHAPTER IN A

### Monograph

1. Bojan Nemec, Nejc Likar, Andrej Gams, Aleš Ude, "Adaptive human robot cooperation scheme for bimanual robots", In: Jadran Lenarčič (ed.), Jean-Pierre Merlet (ed.), *Advances in robot kinematics 2016*, 2018, 371-380.

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1. Igor Kovač, *Cardan joint*, W02018197439 (A1), World Intellectual Property Office, 01. 11. 2018.

### MENTORING

- 1. Aljaž Kramberger, *Autonomous learning of robot actions in contact with the environment:* doctoral dissertation, Ljubljana, 2018 (mentor Aleš Ude).
- 2. Robert Šket, *Physical inactivity related changes in human fecal microbiota:* doctoral dissertation, Ljubljana, 2018 (mentor Blaž Stres; co-mentor Tadej Debevec).

# 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.

The basic and applied research in 2018 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 the direction of the atmospheric variables modelling with Gaussian-process models. The main focus was on the Gaussian-process modelling method and the processing of very large amounts of measurement data.



The second topic was advanced control. We have continued the research and development of model predictive Dr. Gregor Dolanc control (MPC) methods based on fast online optimization, with an emphasis on the fast-gradient method. For the dual fast-gradient method, which we are using for the plasma current and shape controller for the ITER tokamak fusion reactor, we have found an improved method of soft-constraints implementation with a reduced computational load, and analytically determined local convergence rates of the algorithm. With the implementation of the optimisation method using FPGA we have reached a computation time of 1 ms, which is sufficiently short for a practical implementation. Based on the primal fast-gradient method we have designed an improved MCP controller for the stabilization of the unstable resistive wall modes for ITER (Figure 1).

Within the framework of prognostics and health management, substantial progress was achieved in the field of fuel-cell diagnostics in 2018. Together with partner institutions within the INSIGHT project, we implemented an embedded system for data acquisition on an experimental system in CEA, France. On the bases of collected data, we developed several algorithms for feature extraction from fuel-cell impedance spectra. From the collected data, i.e., the parameters of equivalent circuit models, we will continue to develop an expert diagnostic system.

In the area of tools and building blocks for implementation we continued the design of the tool for the analysis and optimization of production performance. In 2018, we continued with work on the problem of material-resource planning. The research was focused on the planning problem where the due date and grouping constraints have to be considered. We have proposed more problem formulations described as an integer-programming problem, which can be applied for various situations that can appear in industry. The method was verified on the data sets from an industrial environment.

In the course of the three-year programme Gostop - Building Blocks, tools and systems for factories of the future we performed activities on both programme management as well as within the framework of R&D projects, where we participated in a number of R&D areas. In the area of the development of the prototype products for smart factories of the

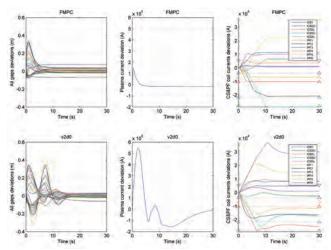
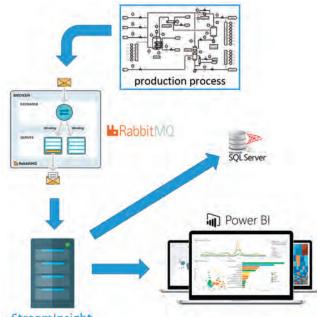


Figure 1: Simulation performance comparison between the MPC plasma current and shape control (top) and the reference CREATE v2d0 scheme (bottom): minor disturbance at t = 520 s. Left: plasma edge geometrical descriptors, centre: plasma current, right: poloidal field coil currents (dotted lines: constraints, with triangles marking their directions)

future, we participated in the development of two prototypes. First, a prototype module to provide 100% quality in a series of finished products on an example of an EC motors production line, and second, a prototype unit for remote process supervision and for the transfer of data from industrial devices through 4th-generation mobile networks. In the area of the development of a platform for the synthesis of models based on the production data, aimed at production process supervision, adaptive control and decision support, we developed the data analytics supporting modules, which were implemented in various analytical environments, in the form of web-services. In this R&D area, we also participated in building an architecture for the processing of complex data. In the area



StreamInsight Figure 2: The architecture of the environment for complex data

processing

of the development of an intelligent tool-management system, we defined a concept for some key components of the system (Figure 2). In the area of the development of the platform for an adaptive correction of the final product quality in the production of EC motors, we assessed the effect of the balancing parameters on the vibrations in the final product. In the area of the development of an experimental concept for an intelligent drive, we took part in the definition of the concept for the drive assemblies, in the definition of the algorithms for the control of torque and compliance and for the predictive maintenance of the drive assembly. We also took part in ensuring the connectivity of the drive assembly, according to the IoT concept, through the development of a specific Linux operating system, using the Yocto environment.

Applied research in the priority problem domains was the third sub-area of our interest. For the Slovenian Research Agency project *Method for the forecasting of local radiological pollution of atmosphere using Gaussian processes* models most of the activities were comprised of the evaluation of different Gaussian-process-based modelling methods for the identification of models useful for forecasting atmospheric variables. Dynamic models for wind and temperature profiles were identified.

Within the *State-of-health estimation of electrochemical energy systems* project, funded by the Slovenian Research Agency, two research tracks were executed in the last year of this project. The first one was focused on the development of time-domain fractional order identification methods with the purpose of implementing prognostics and health-management

tasks. The second track was addressing the stochastic nature of the impedance data. The goal is to employ stochastic decision making for threshold selection and fault isolation. The experimental work is performed on the developed test beds as well as exploiting data from various ongoing H2020 projects in the area of fuel cells.

Following the initiative of the Republic of Slovenia for the establishment and operation of Strategic Innovative Partnerships within the framework of the Slovenian Smart Specialisation Strategy S4, the Strategic Innovative Partnership *Factories of the Future - SRIP ToP* is also operating. Our department has a very active role in SRIP ToP in the management of the area Control Technologies and in the implementation of the Multi-Annual Action Plan of this area. In 2018, a total of 38 Slovenian companies and academic institutions were gathered in this partnership, an implementation action plan was prepared, and a conference was organised where stakeholders were informed about the action plan and the possibilities for participation in its implementation.

#### International R&D projects

The scope of an international project H2020 *Memphys - MEMbrane based Purification of HYdrogen System* 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 task of the Department of Systems and Control is the design of the hardware and the software for the control and diagnostic system. In the last year we finalized the experimental setup (Figure



Figure 3: The experimental setup for the Memphys project.

3), developed and tested the control, diagnostic and condition monitoring algorithms and started with the development of a special electronic unit for fast data acquisition, control and diagnostics.

In cooperation with leading academic and industrial partners in the field of solid-oxide fuel cells (SOFCs), we implement the three-year H2020 project *INSIGHT*. The project is aimed to develop the efficient tools for the on-line health monitoring of SOFC stacks, detection and isolation of the evolving degradation mechanisms and design of the accommodation actions. The IJS team contributes an innovative approach to the characterisation of SOFCs based on the dynamic response to the persistently excited stack and the identified mathematical model in terms of the lumped fractional order differential equations.

This year, in cooperation with TU Graz, Austria, we acquired a new bilateral research project that began in December 2018 to continue the ongoing successful cooperation in the field of fuel-cell fuel-status estimation. During 2018 we carried out some sustainable tests where we deliberately

initiated the degradation processes in fuel cells. On the basis of the obtained results, we improved the system for data acquisition and algorithms for their processing.

In 2018 we also collaborate in a new international project IAPUNIT, which is being implemented within the framework of the *European Defence Agency* (EDA). The project aims to develop an auxiliary fuel source for the fuel cells for military vehicles using F-34 military diesel fuel. This fuel is particularly problematic for usage in fuel cells due to impurities and, accordingly, an adjustment of the fuel processor's design is needed. The motivation for the project is to increase the energy efficiency, reduce noise levels, reduce thermal footprint and reduce pollution – all this in comparison to existing conventional diesel generators.

### Applied work

In the course of a long-term collaboration with Danfoss Trata d.o.o., in 2018 we completed the development of hardware and software for the family of pressure-valve drives. The developed drives are able to automatically detect and reduce oscillations in the system by reducing the operating pressure. For Danfoss we also developed a prototype of a non-linear, highspeed drive and conducted a study of the indirect measurement of fluid flows based on some other physical quantities.

For the Domel Company, Železniki, Slovenia, we designed and built a semi-automatic diagnostic system for the end-of-line control of electric drives for bicycles of the Pedelec type (Figure 4). The mechanical part of the machine consists of two electrically driven helical bevel gear units for simulation of the driving torque and load, and of a manipulator to hold the unit under test during the operation. The diagnostic procedure consists of electrical tests of the control and communication loops, calibration of the internal sensors, encrypted programming of parameters, short run-in, test of torque assistance at several levels and speeds, free-run test, braking operation and safety functions. Also, vibrational tests are made in the range



Figure 4: Diagnostic system for End-of-line control of electric drives for bicycles of the Pedelec type (Pedal Electric Cycle)

up to 5 kHz to detect unbalance of the motor, bearing or transmission problems. All measurements, measurement conditions and diagnostic results are saved into the data servers of the company.

In the field of wastewater treatment, we have started a study for the Kranj wastewater treatment plant, where the aim is to improve the settling of the sludge. Improper sludge settling is associated with the growth of filamentous bacteria and can lead to poor effluent quality. In the study, we analyse the plant's operating conditions, which potentially lead to the growth of filamentous bacteria, for example, high biomass concentration and sludge age, a low oxygen concentration in aerobic reactors, influent composition, etc. The analysis is performed by the developed mathematical model of the plant, data mining and by performing the changes to operational parameters directly on the process.

#### 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.

### Some outstanding publications in the past year

- Boškoski, Pavle, Debenjak, Andrej, Mileva Boshkoska, Biljana. Rayleigh copula for describing impedance data - with application to condition monitoring of proton exchange membrane fuel cells. *European journal of operational research*, ISSN 0377-2217. [Print ed.], 2018, vol. 266, no. 1, pp. 269-277 [COBISS. SI-ID 30736167]
- Gerkšič, Samo, Pregelj, Boštjan, Perne, Matija, Ariola, M., De Tommasi, Gianmaria, Pironti, Alfredo. Model predictive control of ITER plasma current and shape using singular-value decomposition. *Fusion engineering and design*, ISSN 0920-3796. [Print ed.], 2018, vol. 129, pp. 158-163, [COBISS.SI-ID 31239463]
- Glavan, Miha, Gradišar, Dejan, Humar, Iztok, Vrančić, Damir. Refrigeration control algorithm for managing supermarket's overall peak power demand. *IEEE transactions on control systems technology*, ISSN 1063-6536. [Print ed.], 2018, [COBISS.SI-ID 31573799]
- 4. Vrečko, Darko, Nerat, Marko, Vrančić, Damir, Dolanc, Gregor, Dolenc, Boštjan, Pregelj, Boštjan, Meyer, Fabien, Au, Siu Fai, Makkus, Robert, Juričić, Đani. Feedforward-feedback control of a solid oxide fuel cell

power system. International journal of hydrogen energy, ISSN 0360-3199. [Print ed.], 2018, vol. 43, no. 12, pp. 6352-6363, [COBISS.SI-ID 31267367]

5. Nerat, Marko, Juričić, Đani. Modelling of anode delamination in solid oxide electrolysis cell and analysis of its effects on electrochemical performance. International journal of hydrogen energy, ISSN 0360-3199. [Print ed.], 2018, vol. 43, no. 17, pp. 8179-8189, [COBISS.SI-ID 31331367]

### Some outstanding achievements in the past year

- Our department is a partner in the project IAPUNIT Development of an innovative auxiliary power 1 unit for military purposes based on high-temperature PEM fuel cell and reforming technology based on military logistic consumable materials for the European Defence Agency EDA
- 2. European Patent Office approved the patent Reducing oscillations in a control system: patent EP 2356522 B1 to members of our department, dr. Janko Petrovčič and doc. dr. Damir Vrančić.
- For the company Domel doo, Železniki we developed and put into operation a diagnostic system for 3. electric bicycle drives
- 4. The Technology Network Advanced Control Technologies award for the best master thesis in 2018 was granted to Matic Knap for his work entitled Simulation of magnetic plasma shape control in ITER tokamak that was carried out on our department under the mentorship of dr. Samo Gerkšič.

### INTERNATIONAL PROJECTS

- H2020 MEMPHYS; Membrane based Purification of Hydrogen System 1. Dr. Gregor Dolanc European Commission
- H2020 INSIGHT; Implementation in Real SOFC Systems of Monitoring and Diagnostic 2.
- Tools Using Signal Analysis to Increase their Lifetime Prof. Đani Iuričić European Commission
- Health Monitoring and Lifetime Prediction of Solid Oxide Fuel and Electrolysis Cells 3. Prof Đani Iuričić Slovenian Research Agency
- 4. Non-invasive Condition Monitoring of High Temperature Steam Electrolyser Prof. Đani Iuričić

Slovenian Research Agency

### RESEARCH PROGRAM

1. Program systems and control Prof. Đani Juričić

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

1. On-line Degradation Monitoring for Extended Durability of High Temperature Steam Electrolysers Prof. Đani Juričić

### VISITORS FROM ABROAD

- Armando Salvati, University of Salerno, Fisciano (SA), Italy, 16 March 2018 1
- Pietro De Stefano, University of Salerno, Fisciano (SA), Italy, 20 April to 17 July 2018 2. Shambu Nath Sharma, National Institute of Technology, Surat, India, 20 May to 3.
- 20 June 2018 Matija Dubravac, Bjelovar University of Applied Sciences, Bjelovar, Croatia, 2 July to 31 4 August 2018

### STAFF

#### Researchers

- Dr. Pavle Boškoski
- 2. Dr. Gregor Dolanc, Head
- Dr. Samo Gerkšič 3.
- 4. Dr. Giovanni Godena
- Dr. Dejan Gradišar 5.
- 6. Dr. Nadja Hvala Dr. Vladimir Jovan
- Prof. Đani Juričić 8.
- 9. Prof. Juš Kocijan

- Degradation monitoring and performance optimisation of solid oxide electrolysis cells 2 Prof. Đani Iuričić
- 3 State-of-health prognostics of electrochemical energy systems Dr Pavle Boškoski
- 4 E-maintenance of electro-mechanical drives: prognostics and health management solutions under non-stationary operating conditions Prof. Đani Juričić
- 5. Method for the forecasting of local radiological pollution of atmosphere using Gaussian process models
- Prof. Juš Kocijan 6. Building blocks, tools and systems for the Factories of the Future - GOSTOP Dr. Vladimir Jovan
- Ministry of Education, Science and Sport Development of the Control System for the Gas Fuel Processor / Fuel Cell System (Phase

Dr. Gregor Dolanc Frauenhofer-gesellschaft zur Foerderung der

### NEW CONTRACTS

- Development and implementation of the device for bicycle electric drives testing Dr. Janko Petrovčič Domel, d. o. o.
- Quality inspection device for Pedelec eBike Dr. Janko Petrovčič Domel, d. o. o.
- 3. Development of new drive "Flat Station" Asst. Prof. Damir Vrančić Danfoss Trata, d. o. o
- Vanja Subotić, Technische Universität Graz, Graz, Austria, 13-14 September 2018
- 6. Cagla Kuru, Dogus University, Istanbul, Turkey, 1 October 2018 to 31 March 2019
- Muzaffer Oyan, Dogus University, Istanbul, Turkey, 1 October 2018 to 31 March 2019 Jovan Stefanovski. Ss. Cyril and Methodius University in Skopje, Skopje, Macedonia, 24-27 October 2018
- 9. Allard van Baalen, HyET, Arnhem, Netherlands, 18 November to 23 December 2018
- 10. Dr. Bojan Musizza, left 01.11.18
- 11. Dr. Marko Nerat
- 12. Dr. Matija Perne
- 13. Dr. Janko Petrovčič
- 14. Dr. Boštjan Pregelj
- 15. Asst. Prof. Damir Vrančić
- 16. Dr. Darko Vrečko Postdoctoral associates
- 17. Dr. Andrej Debenjak, left 01.05.18
- 18. Dr. Boštjan Dolenc

19. Dr. Miha Glavan

Postgraduates

20. Tomaž Kos, B. Sc. 21. Tadej Krivec, B. Sc.

22. Gjorgji Nusev, B. Sc.

23. Martin Stepančič, B. Sc.

24. Luka Žnidarič, B. Sc.

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# ARTIFICIAL INTELLIGENCE LABORATORY

The Artificial Intelligence Laboratory (http://ailab.ijs.si/) is concerned mainly with the research and development of information technologies, with an emphasis on artificial intelligence. 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 analyzing the scientific community; Enrycher (http://enrycher.ijs.si/), a system for semantic enrichment of textual Head: data; SearchPoint (http://searchpoint.ijs.si/), a portal for visual and contextualized Web browsing; Prof. Dunja Mladenić OntoPlus, a methodology for semi-automatic ontology extension; Contextify (http://contextify. net/), a tool for contextualized e-mail and contact management; Ominer (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; EventRegistry (http://eventregistry.org/), a system for identifying world events in news media; Wikifier (http://

wikifier.org), web service that takes a text document as input and annotates it with links to relevant Wikipedia concepts; StreamStory (http://streamstory.ijs.si), an exploratory datastream analysis tool offering an alternative type of visualization by representing the multivariate data stream using a Markovian model; Videolectures Explorer (http://explore.videolectures. net/), a tool enabling users to search through videolectures and find similarities between them; EDSA dashboard (http:// jobs.videolectures.net/), a tool aggregating demand data (job

A paper entitled "Trading on Talent: Human Capital and Firm Performance", co-written by James Hodson, a member of the AILab and a PhD student within the BigDataFinance ITN, received Best Paper on Long-term Investment Sponsored by Caisse de dépôt et placement du Québec

postings around Europe) and supply data (training materials) in data science; nextPin, a system for the analysis of time-varying data of geographic locations; infominer a system for semi-automatic document analysis; Connection tool (http://connection.ijs.si), a tool based on Event Registry news data, which allows a user to follow business and personal named entities in time and establish broad relations between named entities (based on shared Wikipedia concepts from news articles) as well as to view the changes in these relations; Graph Based Analytics (http://gba.ijs.si) a service for business-relation identification from text that enables the identification of business relations, such as mergers & acquisitions, bankruptcy, earnings, dividends, etc., based on sentence level; streamfusion, universal system for the preprocessing of heterogeneous stream data and ELEXIS ER (http://er.elex.is/), lexicography-adapted version of Event Registry. 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 16 years, members of the Artificial Intelligence Laboratory have successfully participated in 65 EU projects, of which 2 were concluded in 2018 and 15 were still ongoing. In 2018, we were also involved in 6 national projects and 2 industrial projects, with successful collaborations involving the companies Iskratel and Sogeti.

In 2018, in the area of statistical data modelling and machine learning, we successfully concluded the EU H2020 project OPTIMUM (Multi-source Big Data Fusion Driven Pro-activity for Intelligent Mobility). The project demonstrated the use of analytical tools and services in traffic and mobility. Within the project, we built a scalable big-data traffic-infrastructure platform that serves more than 40 traffic-related APIs with data from Slovenia and the EU, and developed a personal pattern detection and prediction service. At the same time, three new EU H2020 projects

focused on the area of **statistical data modelling and machine learning** began in January 2018: *TheyBuyForYou*, *DataBench* and *Perceptive Sentinel*. The EU H2020 project **TheyBuyForYou** (*Enabling procurement data value chains for economic development, demand management, competitive markets and vendor intelligence*) aims at developing methods for analyzing public procurement and the spending of public money in order to ensure greater transparency in the use of public funds and to prevent corruption or other irregularities. In the past year,

## Marko Grobelnik was named member of the OECD Expert group on AI (AIGO).

our work on the project involved the collection and preparation of data on public procurement and public spending data. We have been developing methods for the multilingual comparison of documents - public procurement contracts. We continued our work on the development of algorithms that search for anomalies in financial flows (public-sector payments).

Our work will continue with the development of an online application for visualizing the use of public funds, the analysis of public procurement and the visualization of discovered anomalies. The EU H2020 project DataBench (Evidence Based Big Data Benchmarking to Improve Business Performance) has, as its main goal, the design of a benchmarking process helping European organizations developing BDT to reach for excellence and constantly improve their performance by measuring their technology development activity against the parameters of high business relevance. DataBench will investigate existing Big Data benchmarking tools and projects, identify the main gaps and provide a robust set of metrics to compare technical results coming from those tools. The aim of the EU H2020 project Perceptive Sentinel (BIG DATA knowledge extraction and re-creation platform) is to build a machine-learning framework that will enable efficient data processing on top of Big Data, acquired by satellites from the Sentinel-1, -2 and -3 missions. In the past year, our work on the project was dedicated to performing an initial analysis of the data. Based on preliminary findings, we have, together with our partners, developed an open-source library, EO-learn, and exposed the power of imagery processing and machine learning to a broad set of stakeholders (from students to scientists). We proceeded with the development of feature-extraction algorithms dedicated mostly to the usage of EO-learn in agriculture and with the integration of fast on-line machine-learning methods into the platform. The EU H2020 project Cog-Lo (Cognitive Logistics) started in June 2018. The aim of the project is to design and develop an intelligent logistics platform with cognitive services for postal operators/infrastructure. The project

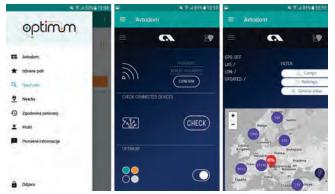


Figure 1: Integration of the MACH web app into the OPTIMUM routing app. Left: tab "Motorhome" ("Avtodom" in Slovenian) appears only if the user connects to the MACH hotspot. Middle and right: example of settings and POI search functionalities. POI search shows current GPS status, latitude, longitude, time, filters for filtering POIs and POIs source, current motorhome location (red marker), nearby POIs list (below the map).

focuses on observing the postal infrastructure as an object in time, with dynamic parcel (packets) flow being driven through basic infrastructural tools. The cognitive services platform will utilize infrastructure data to build a digital representation and dynamically route/allocate assets for process performance optimization. In 2018, we have successfully completed the second year of the EU H2020 EU PrEstoCloud (Proactive Cloud Resources Management at the Edge for Efficient Real-Time Big Data Process ing). The main objective of PrEstoCloud is to create substantial research contributions to the modern environments of edge- and cloud-computing systems in order to provide a dynamic, distributed architecture for proactive resource management. To this end, the PrEstoCloud solution reaches the extreme edge of the network for efficient data processing during run-time. In this project, we are building a service within the PrEstoCloud platform that is responsible for the Mobile Offloading Processing Microservice. This functionality provides the orchestration of services from edge nodes to cloud resources and vice versa. The H2020 EU project enviroLENS (Copernicus for environmental law enforcement support) started in December 2018. The aim of the project is to assist the personnel working in the area of environmental legal issues (legal firms, non-governmental

organizations, etc.) with the discovery of environment-related issues within legislation and other legal documents and to explore potential solutions for finding facts within the remote-sensing/earth-observation (EO) domain. We will build large document exploratory analysis tools and active learning algorithms to enable the faster discovery of the relevant parts of text. These results will later be used in the automatic discovery of spatio-temporal rules within the legislation, which will assist semi-automatic proof discovery using EO data. In 2018, we also concluded the ARRS project **TOPREP** (*Learning Topological Representations*), which is the result of a second-round ERC starting-grant proposal. The goal of the project was to not only identify clusters based on local structure called strata, but also how they fit together using computational topology. This has applications in machine learning and is especially important for time-varying systems, where tipping points can be thought of as the meeting point between two strata. In 2018, the project had several notable research results that combine computational topology with continuous optimization, which has opened up a new area of incorporating topological techniques into deep neural networks. As a part of our activities in the project with Sogeti, we collaborated in a **EUROSTAT Smart**  Statistics project. Our main role was the development of smart-mobility statistics PoC and smart-labour-market statistics PoC. In particular, we performed the following activities: (1) identification of functional, operational and technical requirements related to smart-mobility statistics PoC and smart-labour-market statistics PoC, (2) defining relevant policy areas and policy questions for smart-mobility statistics PoC and smart-labour-market statistics PoC, (3) defining statistical outputs, (4) the implementation of smart-mobility statistics PoC and smart-labour-market statistics PoC and smart-labour-market statistics PoC and smart-labour-market statistics PoC and (5) preparing a roadmap for recommendations to national statistical offices.

In the areas of **text and network analysis and language technologies**, we started the EU H2020 project **SIL-KNOW** (*Silk heritage in the Knowledge Society: from punched cards to big data, deep learning and visual/tangible simulations*). Within the project our work is mainly related to developing methods and services for multilingual big-data text analytics. We are also coordinating the EU H2020 project **ELEXIS** (*European Lexicographic Infrastructure*) that started in February 2018. The aim of the project is to integrate, extend and harmonize national and regional efforts in the field of lexicography, both modern and historical, with the goal of creating a sustainable infrastructure that will (1) enable efficient access to high-quality lexical data in the digital age, and (2) bridge the gap between more advanced and lesser-resourced scholarly communities working on lexicographic resources. In

the past year, in addition to the activities related to project management, we set up the project infrastructure (server and tools); collected, wikified and babelfied the UD- and TenTen corpora for all 14 participating languages, prepared the prototype infrastructure for semantic annotation tasks, and organized an introductory project event for project partners in Ljubljana (February 2018). We also set up the lexicography-adapted version of Event Registry at <u>er.elex.is</u>. Within the EU H2020 Marie Skłodowska-Curie ITN project **BigDataFinance** (*Training for Big Data in Financial Research*)

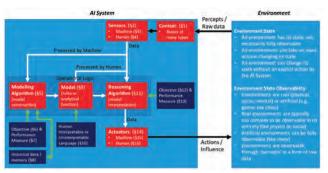
We have successfully concluded two EU H2020 projects: EDSA (*European Data Science Academy*) (http://edsa-project.eu/), OPTIMUM (*Multisource Big Data Fusion Driven Proactivity for Intelligent Mobility*) (http://www.optimumproject.eu/)

and Risk Management) two doctoral students continued to work on topics related to text-data analysis in connection to financial data: "Deep Knowledge Extraction from Financial, Business, and Social Text" and "Characterising Financial Markets from Event-driven Perspective". In 2018, BigDataFinance did not organize any events or conferences, but one of the students chaired the Project Showcase track at the KDD conference in London, UK. The KDD conference is one of the most renowned conferences on Machine Learning and AI. The other doctoral student completed a secondment in London, UK with the financial services firm Bloomberg LP, which is the leading provider of financial data and news in the world. Finally, a paper written by one of the students received an award for the Best Paper on Long-Term Investments from the Northern Finance Association. We are also leading the ARRS project New grammar of contemporary standard Slovene: sources and methods, which began in 2017. The project aims to explore linguistic methodological foundations of a complex analysis of written and spoken Slovene, as found in the new corpora developed in recent projects. The resulting methodology and data will provide a sound foundation for future work on an empirically based description of Slovene. Following from the methodology, we intend to compile and publish extensive collections of extracted material from corpora that will be useful for the development of language-technology applications for Slovene. The extracted data will be used for the linguistic analysis of real language, which represents the first step towards the compilation of a new descriptive corpus grammar of Slovene. In line with these goals, in the last year, we participated in the design and development of several tools for lexical data extraction from text corpora (morphology, wordlists, collocations, multi-word expressions, n-grams), and their related analysis. 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 also contributed various types of data (lexical resources, corpora, training corpora) and technologies (grammatical annotation, lexical data mining) for Slovene language processing.

In the area of **semantic technologies**, the team's work has focused on three European projects. Within the EU H2020 Marie Skłodowska-Curie RISE project **RENOIR** (*Reverse engineering of social information processing*), we completed four secondments to Stanford University and Carnegie Mellon in the US. Our work in 2018, focused on research activities combining machine-learning methods and social network analysis for the reverse engineering of social information processing. The long-term goal is developing methods for the automated collaboration of never-ending learning systems and testing the approach on two existing never-ending learning systems, one for language learning and the other for event learning, both requiring social information processing. Work was also done on how to continuously optimize topological structure in the spectral domain. The EU H2020 project **euBusinessGraph** (*Enabling the European Business Graph for Innovative Data Products and Services*) started in January 2017. The aim of the project is to build a European cross-lingual "business graph" that will aggregate, link and provision high-quality company-related data. In the past year, our work on the project consisted of collecting

and preparing the data of companies, which we included in our Wikifier tool. We developed a methodology along with tools and services that provide analytics functionalities for named entities, such as people and organizations, on top of business news. We have prepared a service for establishing business relationships from text and integrated Event Registry services into euBusinessGraph business cases and the marketplace. As members of the EU H2020 innovation action project **EW-Shopp** (*Supporting Event and Weather-based Data Analytics and Marketing along the Shopper Journey*), we are building a toolkit for supporting data-driven e-commerce. This toolkit enables businesses to integrate their data with contextual information about weather and events and use analytics on this data to power their services. We designed and implemented the analytics tool, based on our own QMiner data-analytics platform, which enables businesses to setup a comprehensive machine-learning pipeline to build a model of their data and deploy it as a predictive service. Furthermore, we are contributing to the Event Registry system, which is used as the source of event data. The project has a large number of international business partners including three Slovenian companies - Ceneje.si, Big Bang and CDE.

In the area of knowledge management, the group's main focus includes research and development by using methods and tools from a broader Artificial Intelligence area in real business settings. The EU H2020 project EDSA (European Data Science Academy), was successfully concluded in 2018. Within the project, we contributed



*Figure 2: Detailed conceptual view to AI with references to individual elements developed by Marko Grobelnik as part of the OECD AIGO AI Definition.* 

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, in particular videolectures from the VideoLectures.NET portal. We also participated in the EDSA curriculum development, developing and maintaining training and learning analytics applications based on Videolectures.NET data, such as the 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). The EU H2020 project x5gon (Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross *Site Global OER Network*) is at its midpoint. The goal of the project is to implement innovative technology elements for connecting scattered Open Educational Resources (OERs) available across Europe and the globe. Our department, in collaboration with the Centre for Knowledge Transfer in Information Technologies (CT3), has developed a pipeline for processing multimodal data (text, video and audio materials) and developed a system

for accessing this data within the platform. In addition, we have also developed a preliminary version of rich material and user models that are used for providing the personalized recommendation of learning materials as well as a search web application for finding OER materials (https://platform.x5gon.org/search). In collaboration with the Centre for Knowledge Transfer in Information Technologies (CT3), the EU H2020 project MOVING (TraininG towards a society of data-saVvy inforMation prOfessionals to enable open leadership INnovation) is in its final year. We were mostly active in producing video demonstrations about the developed technologies, services and the MOVING platform, for the purpose of dissemination and exploitation activities. The videos also serve for the didactic and curricula development in the MOVING platform, that enables its users to improve their information literacy by training how to exploit data-mining methods in their daily research tasks. In 2018, together with the Centre for Knowledge Transfer in Information Technologies (CT3), we continued with the EU H2020 RISE project Water4Cities (Integrated surface and groundwater management for sustainable urban development). We continued to collect and analyse data on the example of Ljubljana and the Greek island of Skiathos, with the help of which we are developing models and a platform that will enable the monitoring of urban water resources in real time. This will contribute to optimal water management and minimize environmental and ecosystem impacts. In 2018, we recorded a special session dedicated to the Water4Cities project at the EWAS conference. We also video record and edit regular webinars and interviews with researchers involved in the project. All the recordings are hosted on the Videolectures.NET portal.

**Promotion of science** is continuously present in the efforts of the Artificial Intelligence Laboratory. In 2018, members of the Artificial Intelligence Laboratory were very active in promoting this research topic. Marko Grobelnik, Dunja Mladenić, Zala Herga and Simon Krek gave a total of 8 interviews related to the topic of Artificial Intelligence:

- Marko Grobelnik was a guest speaker on National RTVSlo show Turbulenca
- An interview with Marko Grobelnik aired for the Slovenian radio Val202.
- An interview with Marko Grobelnik aired on Radiotelevizija Slovenija javni zavod, Prvi
- Marko Grobelnik gave an interview for the Slovenian magazine Mladina

- Marko Grobelnik was a guest speaker on Studio City Artificial Intelligence
- Dunja Mladenić gave an interview for *The Slovenia Times* Slovenia, putting artificial intelligence in medicine to work
- Zala Herga gave an interview regarding the EU H2020 project OPTIMUM on Ljubljana TV.
- Simon Krek gave an interview promoting the new EU H2020 project ELEXIS in the national newspaper *Delo*.

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 2018, 176 students from 28 schools participated in the competition. We have also been organizing a touring exhibition about female PhD holders from the area of computer science in Slovenia since 2006, thereby promoting the role of women in science (http://ScienceWithArt.ijs.si/).

In 2018, we were very actively involved in submitting new project proposals, particularly within the EU H2020 Programme. Once again, we were very successful, obtaining funding for five new projects: *Cleopatra*, *FinTech*, *NAIADES*, *HumaneAI*, and *CyberSANE*. We continue with our successful efforts to include Slovenian industry in the European research area, where over the last 16 years we have produced a list of numerous companies participating in EU projects.

#### Some outstanding publications in the past year

- Kenda, Klemen, Mladenić, Dunja. Autonomous sensor data cleaning in stream mining setting. *Business systems research journal : international journal of the Society for Promotion of Business Information Technology (BIT)*, ISSN 1847-8344, 2018, vol. 9, no. 2, str. 69-79, doi: 10.2478/bsrj-2018-0020. [COBISS. SI-ID 31531815], [WoS do 10. 8. 2018: št. citatov (TC): 0, čistih citatov (CI): 0, Scopus do 8. 12. 2018: št. citatov (TC): 0, čistih citatov (CI): 0, šistih citatov (CI): 0]
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personality profiles to nudge for sustainable transportation. Journal of intelligent information systems, ISSN 0925-9902, [in press] 2018, pg. 22.

#### Awards and Appointments

 James Alexander Hodson: Best Paper on Long-term Investment, Northern Finance Association 2018 (NFA 2018), 21 – 23 September 2018, Charlevoix, Canada, Trading on Talent: Human Capital and Firm Performance

#### Organization of Conferences, Congresses and Meetings

- 1. H2020 Elexis project meeting, Ljubljana, Slovenia, 15 17 February 2018
- 2. H2020 X5Gon workshop, Ljubljana, Slovenia, 16 20 April 2018
- 3. H2020 TheyBuyForYou project meeting, Bled, Slovenia, 8 9 May 2018
- 4. H2020 DataBench workshop, Cerkovnik, Slovenia, 19 20 May 2018
- 5. H2020 DataBench project meeting, Bled, Slovenia, 21 22 May 2018
- 6. Workshop Nova slovnica: viri in metode, Ljubljana, Slovenia, 6 June 2018
- 7. wnlex Wordnet as Lexicographical Resource workshop, Ljubljana, Slovenia, 17 July 2018
- 8. Seminar K Dictionaries & Lexicala, Ljubljana, Slovenia, 17 July 2018
- 9. H2020 RENOIR project meeting, Ljubljana, Slovenia, 26 28 September 2018
- 10. IW3C meeting, Ljubljana, Slovenia, 17 20 October 2018

## INTERNATIONAL PROJECTS

1.	INEA/CEF - eTranslation TermBank
	Dr. Simon Krek
	Innovation And Networks Executive Age
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- Innovation And Networks Executive Agency (inea)
   INEA/CEF MARCELL, Multilingual Resources for CEF.AT in the Legal Domain Dr. Simon Krek
- Innovation And Networks Executive Agency (inea)
- COST CA16105; European Network for Combining Language Learning with Crowdsourcing Techniques Dr. Simon Krek

Cost Office

- 4. H2020 EDSA; European Data Science Academy Marko Grobelnik
- European Commission
- H2020 OPTIMUM; Multi-source Big Data Fusion Driven Proactivity for Intelligent Mobility
- Marko Grobelnik
- European CommissionH2020 BigDataFinance; Training for Big Data in Financial Research and Risk Management
- Marko Grobelnik
- European Commission
- H2020 RENOIR; Reverse Engineering of Social Information Processing Marko Grobelnik
- European Commission
- H2020 MOVING; Training Towards a Society of Data-Savvy Information Professionals to enable Open Leadership Innovation Marko Grobelnik
- European Commission
- H2020 PrEstoCloud; Proactiive Cloud Resources Management at the Edge for Efficient Real-Time
- Marko Grobelnik
- European Commission
- H2020 euBusinessGraph; Enabling the European Business Graph for Innovative Data Products and Services Prof. Dunia Mladenić
- European Commission
- H2020 EW-Shopp; Supporting Event and Weather-based Data Analytics and Marketing along the Shopper Journey Marko Grobelnik
- European Commission
- H2020 Water4Cities; Holistic Surface Water and Groundwater Management for Sustainable Cities Marko Grobelnik
- European Commission
- 13. H2O2O X5gon; Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network

Marko Grobelnik European Commission

- 14. H2020 PerceptiveSentinel; BIG DATA Knowledge Extraction and Re-creation Platform Prof. Dunja Mladenić European Commission
- H2020 DataBench; Evidence Based Big Data Benchmarking to Improve Business Performance
  - Marko Grobelnik European Commission
- 6. H2020 TheyBuyForYou; Enabling Procurement Data Value Chains for Economic Development, Demand Management, Competitive Markets and Vendor Intelligence Marko Grobelnik
- European Commission 17. H2020 - SILKNOW; Silk Heritage in the Knowledge Society; From Punched Cards to Big Data, Deep Learning and Visual/Tangible Simulations Prof. Dunja Mladenić
  - European Commission
- H2020 COG-LO; COGnitive Logistics Operations through secure dynamic and ad-hoc collaborative networks
  - Marko Grobelnik European Commission
- H2020 EnvirolENS; Coprenicus for Environmental Law Enforcement Support Marko Grobelnik
- European Commission
- H2020 GlobalDNA; Dynamic Network of Global News Events Prof. Dunia Mladenić
- European Commission
- 21. H2020 ELEXIS; European Lexicographic Infrastructure Dr. Simon Krek European Commission
- Computing Persistent Homology for Geometric Inputs Asst. Prof. Primož Škraba Slovenian Research Agency

### RESEARCH PROGRAM

1. Knowledge Technologies Prof. Dunja Mladenić

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

- Integration of mobile devicas into survey research in social sciences: Development of a comprehensive methodological approach Marko Grobelnik
- Collocation as a basis for language description: semantic and temporal perspectives Dr. Simon Krek
- New modes and Global Patterns of Online News (Re)production Prof. Dunja Mladenić

- 4. Slovene scientific texts: resources and description Dr. Simon Krek
- 5. Learning Topological Representations Asst. Prof. Primož Škraba
- New grammar of modern standard Slovene: resources and methods Dr. Simon Krek
- Forbidden Books in the Slovenian Lands in the Early Modern Period Dr. Simon Krek
- 8. For the Quality of Slovene Textbooks

## VISITORS FROM ABROAD

- 1. Abraham Hsuan, Irwin & Hsuan LLC, New York, USA, 16 23 January 2018
- 2. Michael Witbrock, IBM Research AI, New York, USA, 18 25 January 2018
- 3. Janusz Holyst, Warsaw University of Technology, Warsaw, Poland, 7 15 February 2018
- 4. Dr. John Davies, British Telecom, London, United Kingdom, 28 February 3 March 2018
- 5. Ye Zeng , Aarhus University, Aarhus, Denmark, 28 April 30 June 2018
- 6. M. Besher Massri, Koç University, Istanbul, Turkey, 15 June 15 August 2018
- 7. Dumitru Roman, Sintef, Trondheim, Norway, 21 May 5 June 2018
- 8. Natasha Jaeger, Samsung Research, Laleham, United Kingdom, 19 June 2018
- 9. Steve Park, Samsung Research, Laleham, United Kingdom, 19 June 2018

### STAFF

Researchers

- 1. Asst. Prof. Branko Kavšek\*
- 2. Dr. Iztok Kosem
- 3. Dr. Simon Krek
- 4. Dr. Gregor Leban
- 5. Dr. Jurij Leskovec
- 6. Prof. Dunja Mladenić, Head
- 7. Prof. John Stewart Shawe-Taylor
- 8. Asst. Prof. Primož Škraba
- Postdoctoral associates
- 9. Dr. Kaja Dobrovoljc
- 10. Dr. Blaž Fortuna\*
- 11. Dr. Mario Karlovčec, left 01.04.18
- 12. Dr. Aljaž Košmerlj
- 13. Dr. Inna Novalija
- 14. Dr. Joao Paulo Pita Da Costa
- 15. Dr. Jan Rupnik\*
- 16. Dr. Salman Taherizadeh

#### Postgraduates

- 17. Luka Bradeško, B. Sc., on leave 16.12.17
- 18. Jaka Čibej, B. Sc.
- 19. Rayid Ghani, M. Sc.
- 20. Zala Herga, B. Sc., left 01.11.18
- 21. James Alexander Hodson, B. Sc.
- 22. Mitja Jermol, M. Sc.
- 23. Blaž Kažič, B. Sc

## **BIBLIOGRAPHY**

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- Adrien Poulenard, Primož Škraba, Maks Ovsjanikov, "Topological function optimization for continuous shape matching", *Computer* graphics forum, 2018, 37, 5, 13-25.
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- Evgenia Belyaeva, Aljaž Košmerlj, Dunja Mladenić, Gregor Leban, "Automatic estimation of news values reflecting importance and closeness of news events", *Informatica: an international journal of computing and informatics*, 2018, 42, 4, 527-533.
- 6. Fred Sun Lu *et al.* (13 authors), "Accurate influenza monitoring and forecasting using novel internet data streams", *Journal of medical internet research: JMIR*, 2018, **4**, 1, e4.

Dr. Simon Krek Ministry of Education, Science and Sport

- Strategic Research & Innovation Partnership (SRIP) Smart Cities and Communities Prof. Dunia Mladenić
- Ministry of Economic Development and Technology
- 10. Smart Statistics Marko Grobelnik

Sogeti Luxembourg S.a.

- 10. Brian Song, Samsung Research, Laleham, United Kingdom, 19 June 2018
- 11. Rickard Brüel Gabrielsson, Stanford University, Palo Alto, USA, 22 July 3 August 2018
- 12. Sebastian Peterlin, Stanford University, Palo Alto, USA, 3 September 3 November 2018
- 13. Natasha Jaeger, Samsung Research, Laleham, United Kingdom, 4 September 2018
- 14. Sungmok Seo, Samsung Research, Laleham, United Kingdom, 4 September 2018
- 15. Hojung Lee, Samsung Research, Laleham, United Kingdom, 4 September 2018
- 16. Omar Rashed, , Egypt, 5 October 21 December 2108
- Jasminka Dobša, Pakulteta za organizacijo in informatiko, Univerza v Zagrebu, Varaždin, Croatia, 18 - 19 December 2018
- 24. Klemen Kenda, B. Sc. 25. Erik Novak, B. Sc. 26. Dr. Luka Stopar 27. Miha Torkar, B. Sc. Technical officers 28. Dr. Janez Brank 29. Dr. Miha Cimperman 30. Flavio Fuart, B. Sc. 31. Teja Goli, B. Sc. 32. Dr. Matej Kovačič 33. Mojca Kregar Zavrl, B. Sc. 34. Matej Posinković, B. Sc. 35. Matjaž Rihtar, B. Sc. 36. Mateja Škraba, B. Sc. 37. Dr. Polona Škraba Stanič 38. Jasna Urbančič, B. Sc. Technical and administrative staff 39. Aleš Buh 40. Jasna Franko 41. Marko Grobelnik 42. Monika Kropej, B. Sc.
- 43. Blaž Novak, B. Sc.

Note: \* part-time JSI member

- A.-S. Dadzie Dadzie, E. M. Sibarani, Inna Novalija, Simon Scerri, "Structuring visual exploratory analysis of skill demand", *Journal of web* semantics, 2018, 49, 51-70.
- Nike Kocijančič-Pokorn, Jaka Čibej, ""It's so vital to learn Slovene": mediation choices by asylum seekers in Slovenia", *Language problems* & language planning, 2018, 42, 3, 288-307.
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- 11. Bo Wang, Armin Pourshafeie, Marinka Žitnik, Junjie Zhu, Carlos D. Bustamante, Serafim Batzoglou, Jurij Leskovec, "Network enhancement as a general method to denoise weighted biological networks", *Nature communications*, 2018, **9**, 3108.
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- Salman Taherizadeh, Vlado Stankovski, Marko Grobelnik, "A capillary computing architecture for dynamic internet of things - orchestration

of microservices from edge devices to fog and cloud providers: 2938", *Sensors*, 2018, **18**, 9, 1-23.

- 14. Kaja Dobrovoljc, "Raba tipično govorjenih diskurznih označevalcev na spletu", *Slavistična revija: časopis za jezikoslovje in literarne vede*, 2018, **66**, 4, 497-513.
- Kaja Dobrovoljc, "Formulaičnost v slovenskem jeziku", Slovenščina 2.0: empirične, aplikativne in interdisciplinarne raziskave, 2018, 6, 2, 67-95.
- 16. Nike Kocijančič-Pokorn, Jaka Čibej, "Interpreting and linguistic inclusion friends or foes?: results from a field study", *The Translator: studies in intercultural communication*, 2018, **24**, 2, 111-127.

#### PUBLISHED CONFERENCE CONTRIBUTION

- 1. Salman Taherizadeh, Blaž Novak, Marija Komatar, Marko Grobelnik, "Real-time data-intensive telematics functionalities at the extreme edge of the network: experience with the PrEstoCloud project", In: Sorel Reisman (ed.), *Annual Computer Software and Applications Conference*, 2018 IEEE 42nd Annual Computer Software and Applications Conference, COMPSAC 2018, 23-27 July, 2018, Tokyo, Japan, 2018, 522-527.
- Monika Kalin Golob, Simon Krek, "Terminologija za sodobno sociologijo", In: Miroljub Ignjatović (ed.), Aleksandra Kanjuo-Mrčela (ed.), Roman Kuhar (ed.), Družba in družbena gibanja 50 let po 1968, 2018, 131-134.
- 3. Klemen Kenda, Dimitris Kofinas, Stamatia Rizou, Panagiotis D. Ritsos, Chrysi Laspidou, Nikos Mellios, Matej Senožetnik, "Smart water management for cities", In: Fragile earth: Theory Guided Data Science to Enhance Scientific Discovery: KDD 2018, London, 2018.
- Ramon Iglesias, Federico Rossi, David Hallac, Jurij Leskovec, "Datadriven model predictive control ofautonomous mobility-on-demand systems", In: *ICRA 2018*, 2018 IEEE International Conference on Robotics and Automation, May 21-25, 2018, Brisbane, Australia, 2018.
- Massri M. Besher, Inna Novalija, Marko Grobelnik, "Relation Tracker tracking the main entities and their relations through time", In: Dunja Mladenić (ed.), Marko Grobelnik (ed.), Data mining and data warehouses - SiKDD: proceedings of the 21st International Multiconference Information Society - IS 2018, October 8-12, 2018, [Ljubljana, Slovenia]: volume C, 2018, 13-16.
- 6. Inna Novalija, Marko Grobelnik, "Towards smart statistics in labour market domain", In: Dunja Mladenić (ed.), Marko Grobelnik (ed.), Data mining and data warehouses - SiKDD: proceedings of the 21st International Multiconference Information Society - IS 2018, October 8-12, 2018, [Ljubljana, Slovenia]: volume C, 2018, 9-12.
- Marinka Žitnik, Monica Agrawal, Jurij Leskovec, "Modeling polypharmacy side effects with graph convolutional networks", In: *Proceedindgs of the International Symposium on Biological Monitoring, ISMB 2018, July 6 - July 10, Chicago, IL, USA*, (Bioinformatics 34), 2018, 13, i457-i466.
- Iztok Kosem, Simon Krek, Polona Gantar, Špela Arhar Holdt, Jaka Čibej, Cyprian Laskowski, "Collocations dictionary of modern Slovene", In: Jaka Čibej (ed.), et al., Proceedings of the 18th EURALEX International Congress, [17-21 July 2018, Ljubljana]: lexicography in global contexts, 18th EURALEX International Congress, 17-21 July 2018, Ljubljana, 2018, 989-997.
- 9. Simon Krek, Iztok Kosem, John P. McCrae, Roberto Navigli, Bolette S. Pedersen, Carole Tiberius, Tanja Wissik, "European Lexicographic Infrastructure (ELEXIS)", In: Jaka Čibej (ed.), et al., Proceedings of the 18th EURALEX International Congress, [17-21 July 2018, Ljubljana]: lexicography in global contexts, 18th EURALEX International Congress, 17-21 July 2018, Ljubljana, 2018, 881-891.
- 10. Jaka Čibej, Špela Arhar Holdt, "Researching dictionary needs of language users through social media: a semi-automatic approach", In: Jaka Čibej (ed.), et al., Proceedings of the 18th EURALEX International Congress, [17-21 July 2018, Ljubljana]: lexicography in global contexts, 18th EURALEX International Congress, 17-21 July 2018, Ljubljana, 2018, 67-76.
- 11. Špela Arhar Holdt, Jaka Čibej, Kaja Dobrovoljc, Polona Gantar, Vojko Gorjanc, Bojan Klemenc, Iztok Kosem, Simon Krek, Cyprian Laskowski, Marko Robnik Šikonja, "Thesaurus of modern Slovene: by the community for the community", In: Jaka Čibej (ed.), et al., Proceedings of the 18th EURALEX International Congress, [17-21 July 2018, Ljubljana]: lexicography in global contexts, 18th EURALEX International Congress, 17-21 July 2018, Ljubljana, 2018, 401-410.
- 12. Klemen Kenda, Matej Čerin, Mark Bogataj, Matej Senožetnik, Kristina Klemen, Petra Pergar, Chrysi Laspidou, Dunja Mladenić, "Groundwater modeling with machine learning techniques: Ljubljana polje Aquifer", In: Vasilis Kanakoudis (ed.), Evangelos Keramaris (ed.), Proceedings of

the The 3rd EWaS3 International Conference on "Insights on the Water-Energy-Food Nexus", 27-30 June 2018, Lefkada Island, Greece, 2018, 2, 11, 697.

- 13. Matej Senožetnik, Zala Herga, Tine Šubic, Luka Bradeško, Klemen Kenda, Kristina Klemen, Petra Pergar, Dunja Mladenić, "IoT middleware for water management", In: Vasilis Kanakoudis (ed.), Evangelos Keramaris (ed.), Proceedings of the The 3rd EWaS3 International Conference on "Insights on the Water-Energy-Food Nexus", 27-30 June 2018, Lefkada Island, Greece, 2018, 2, 11, 696.
- 14. Justin Cheng, Jon Kleinberg, Jurij Leskovec, David Liben-Nowell, Bogdan State, Karthik Subbian, Lada A. Adamic, "Do diffusion protocols govern cascade growth?", In: Proceedings of the Twelfth International Conference on Web and Social Media, June 25-28, 2018, Stanford, California, USA, 2018.
- 15. Kaja Dobrovoljc, Matej Martinc, "Er ... well, it matters, right? On the role of data representations in spoken language dependency parsing", In: *Proceedings of the workshop*, Second Workshop on Universal Dependencies (UDW 2018), November 1, 2018, Brussels, 2018, 37-46.
- 16. Jiaxuan You, Rex Ying, Xiang Ren, William L. Hamilton, Jurij Leskovec, "GraphRNN:: enerating realistic graphs with deep auto-regressive models", In: *Reproducibility in machine learning: ICML 2018 - RML* Workshop, July 15, 2018, Stockholm, Sweden.
- 17. Srijan Kumar, William L. Hamilton, Jurij Leskovec, Dan Jurafsky, "Community Interaction and conflict on the web", In: *The Web Conference 2018: proceedings of the World Wide Web Conference WWW2018, April 23-27, 2018, Lyon, France*, 2018.
- 18. Lin Zhiyuan, Tim Althoff, Jurij Leskovec, Dan Jurafsky, "Il'be back: on the multiple lives of users of a mobile activity tracking application", In: *The Web Conference 2018: proceedings of the World Wide Web Conference WWW2018, April 23-27, 2018, Lyon, France*, 2018.
- 19. Emma Pierson, Tim Althoff, Jurij Leskovec, "Modeling individual cyclic variation in human behavior", In: *The Web Conference 2018: proceedings of the World Wide Web Conference WWW2018, April 23-27, 2018, Lyon, France*, 2018.
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- 21. Chantat Eksombatchai, Pranav Jindal, Jerry Zitao Liu, Yunchen Liu, Rahul Sharma, Charles Sugnet, Mark Urlich, Jurij Leskovec, "Pixie: a system for recommending 3+ billion items to 200+ million users in realtime", In: *The Web Conference 2018: proceedings of the World Wide Web Conference WWW2018, April 23-27, 2018, Lyon, France*, 2018.
- 22. Tadej Škvorc, Simon Krek, Senja Pollak, Špela Arhar Holdt, Marko Robnik Šikonja, "Evaluation of statistical readability measures on Slovene texts", In: Darja Fišer (ed.), Andrej Pančur (ed.), Proceedings of the Conference on Language Technologies & Digital Humanities, September 20th - 21st 2018, Ljubljana, Slovenia, 2018, 240-247.
- 23. Kaja Dobrovoljc, "Frekvenčni seznami n-gramov v korpusih slovenskega jezika", In: Darja Fišer (ed.), Andrej Pančur (ed.), Proceedings of the Conference on Language Technologies & Digital Humanities, September 20th - 21st 2018, Ljubljana, Slovenia, 2018, 47-54.
- 24. Polona Gantar, Špela Arhar Holdt, Jaka Čibej, Taja Kuzman, Teja Kavčič, "Glagolske večbesedne enote v učnem korpusu ssj500k 2.1", In: Darja Fišer (ed.), Andrej Pančur (ed.), Proceedings of the Conference on Language Technologies & Digital Humanities, September 20th - 21st 2018, Ljubljana, Slovenia, 2018, 85-92.
- Iztok Kosem, Simon Krek, Polona Gantar, Špela Arhar Holdt, Jaka Čibej, Cyprian Laskowski, "Kolokacijski slovar sodobne slovenščine", In: Darja Fišer (ed.), Andrej Pančur (ed.), Proceedings of the Conference on Language Technologies & Digital Humanities, September 20th - 21st 2018, Ljubljana, Slovenia, 2018, 133-139.
   Polona Gantar, Kristina Štrkalj Despot, Simon Krek, Nikola Ljubešić,
- 26. Polona Gantar, Kristina Štrkalj Despot, Simon Krek, Nikola Ljubešić, "Towards semantic role labeling in Slovene and Croatian", In: Darja Fišer (ed.), Andrej Pančur (ed.), Proceedings of the Conference on Language Technologies & Digital Humanities, September 20th - 21st 2018, Ljubljana, Slovenia, 2018, 93-98.
- 27. Aleksander Ključevšek, Simon Krek, Marko Robnik Šikonja, "Učinkovit izračun frekvenčnih statistik za slovenske jezikovne korpuse", In: Darja Fišer (ed.), Andrej Pančur (ed.), Proceedings of the Conference on Language Technologies & Digital Humanities, September 20th - 21st 2018, Ljubljana, Slovenia, 2018, 126-132.

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A

#### Monograph

- Jaka Čibej, Špela Arhar Holdt, Tomaž Erjavec, Darja Fišer, "Ročno označeni korpusi Janes za učenje jezikovnotehnoloških orodij in jezikoslovne raziskave", In: Darja Fišer (ed.), Viri, orodja in metode za analizo spletne slovenščine, 2018, 44-73.
- Jaka Čibej, "Regionalne jezikovne različice v slovenski računalniško posredovani komunikaciji: korpusni pristop z ročno označenim korpusom Janes-Geo", In: Darja Fišer (ed.), Viri, orodja in metode za analizo spletne slovenščine, 2018, 160-197, 383.

#### **PROFESSIONAL MONOGRAPH**

- 1. Sadhana Singh, Dunja Mladenić, *Expressing leadership and success: based on Kundalini yoga as taught by Yogi Bhajan*, Waldzell: Leadership Institute, 2018.
- Iztok Kosem, Júlia Bálint Čeh, Vojko Gorjanc, Anna Kolláth, Attila Kovács, Simon Krek, Sonja Novak-Lukanovič, Jutka Rudaš, Osnutek

koncepta novega velikega slovensko-madžarskega slovarja, Ljubljana: Univerza v Ljubljani, Filozofska fakulteta, 2018.

## SECONDARY AND PRIMARY SCHOOL TEXTBOOK OR OTHER TEXTBOOK

1. Gregor Anželj, Janez Brank, Andrej Brodnik, Luka Fürst, Matija Lokar, Andrej Brodnik, *Slikovno programiranje: e-učbenik za uvod v programiranje*, Ljubljana: Založba Fakultete za računalništvo in informatiko; Maribor: Založba Fakultete za elektrotehniko, računalništvo in informatiko, 2018.

#### MENTORING

1. Luka Stopar, *Visualizing qualitative patterns in multivariate time series:* doctoral dissertation, Ljubljana, 2018 (mentor Dunja Mladenić; comentor Primož Škraba).

## LABORATORY FOR OPEN SYSTEMS AND NETWORKS E-5

The main activities of the laboratory are R&D in the area of next-generation networks, telecommunications technologies, components and integrated systems, information-society services and applications, especially those that enable better privacy protection for citizens and increased trustworthiness of the information and communication technologies and services.

The research in 2018 was performed within the programme "Future Internet Technologies: concepts, architectures, services and socio-economic issues", funded by the Slovenian Research Agency. In addition, research was carried out in the EU Horizon 2020 projects "Flex4Grid", "Defender" and "Compact", the 7FP project "EmployID", the "SENTER" project from the ISFP programme, the EU DG Justice "LIVE\_FOR" project, the "GIRDA" project from the Erasmus+ programme, the "SI-PASS" and "eID4U" projects from the CEF programme, the "EkoSmart" project from the European regional development fund, and the national "Technological and business aspects of future ecosystem for e-health" project. The focus was the development of technologies and services in advanced next-generation networks, security and privacy in information systems, and technology-enhanced learning.

Members of the laboratory are teaching at the undergraduate and graduate levels at the University of Ljubljana, *Asst. Prof. Tomaž Klobučar* the Jožef Stefan International Postgraduate School, the DOBA Faculty, and the Faculty of Commercial and Business Sciences. In 2018, the Laboratory became a member of European Cyber Security Organisation (ECSO).



Head (since 1. 4. 2018): Asst. Prof. Tomaž Klobučar

#### Concepts and architectures of the secure internet

The first area of research and development was focused on security infrastructures and secure services.

The main goal of the **SI-PASS** ("Slovenian eIDAS node and integrated services") and **eID4U** ("eID for University") projects from the EU CEF (Connecting Europe Facility) programme is to set up an infrastructure for secure cross-border services in different application domains. The SI-PASS project, which is coordinated by the Laboratory for Open Systems and Networks, has established the central eIDAS node in Slovenia at the Ministry of Public Administration and has integrated four public and one private cross-border e-services in the fields of e-health (zVEM), pension and disability insurance (eZPIZ), intellectual property protection, company registers (Portal AJPES), and e-commerce (ePero). The eIDAS node is the central point of trust in the country. On the one hand, it connects the national infrastructure with foreign service providers and, on the other hand, national identity and service providers with the infrastructures of other EU countries.

In the eID4U project we have also linked the test eIDAS node with trusted sources of information about students (central evidence system for e-higher education eVŠ) and various e-learning services. In 2018, the eID4U project analysed the academic attributes needed for Erasmus+ exchanges and developed an XML scheme and the XML definitions of the attributes, upgraded the EU DIGIT reference implementation of an eIDAS node, and developed connectors for several attribute providers. We have created a plugin for the Moodle open-source learning-management system that enables a direct connection to the eIDAS node and learner identity verification using the eIDAS infra-

structure. The results of both projects enable foreigners to access Slovenian e-services with their national notified electronic identification means, and will provide in the near future easy access to public e-services in other EU Member States for Slovenian users.

In the spring of 2018, the project "Prosumer Flexibility Services for Smart Grid management (Flex4Grid)" from the Horizon 2020 EU programme was successfully concluded. The project was part of the call for Competitive low-carbon energy from the Societal Challenges pillar. Based on the innovative use of ICT technologies we have improved the smart-grid operation by utilizing the prosumers flexibility. The project had a strong Slovenian contribution, with Elektro Celje and Smart Com as partners in the project, besides the Jožef Stefan Institute. Slovenian partners were working together to realize a large-scale pilot in the Celje region. The Flex4Grid project has also extended collaboration with Electro Celje in the national Critical Peak Tariff project (CPTP), initiated by the Public Agency of the Republic of Slovenia for energy and financed by SODO. The projects synergy

Head (until 31. 3. 2018): **Prof. Borka Jerman Blažič** 

We have created building blocks for security infrastructures and secure Internet services.

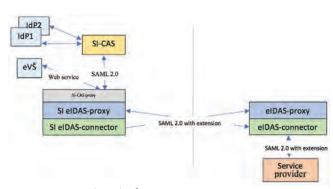


Figure 1: eIDAS node and infrastructure

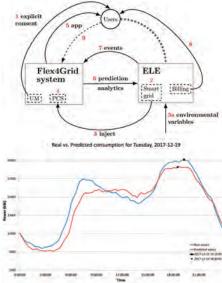


Figure 2: Conceptual model of the Flex4Grid system implementation (above) and comparison between prediction and realization of power consumption in households for a critical peak event (below).

resulted in large-scale piloting in the Celje region with more than 750 test users in a population of 14000 end users. For the projects, we have developed a dynamic energy-consumption forecasting model together with data analytic tools for peak-events evaluation. In the last project phase, in 2018, the CPTP users were enabled with the Flex4Grid home kits to further stimulate their participation in smart-grid flexibility management. The CPT project has extended the pilot operation until the end of 2018.

The **Defender** ("Defending the European Energy Infrastructures") project is addressing the issues of European critical energy infrastructures' security and dependability. The threeyear project aims at improving the protection of all energy-domain segments, from generation, transmission to distribution. The improvements will result in better infrastructure resilience and dependability. The project is the only large-scale project funded through the Horizon 2020 mechanisms that is addressing the critical energy infrastructure protection. Besides a number of excellent European industrial partners, it has a strong Slovenian consortium, namely JSI, Laboratory for Open Systems and Networks together with the Department of Communication Systems, the Slovenian transmission operator ELES and the Institute for Corporative Security Studies (ICS). The laboratory has led the work on cyber-physical threats assessment and analysis and will contribute to the development and implementation of the project threat-mitigation and situation-awareness solutions. The solutions developed in the project will bring together ELES's physical, business and technical security systems and will be tested in the pilot environment of the RTP Okroglo.

The Laboratory members are also involved in a three-year national programme "Ecosystem of a smart city (**EkoSmart**)" with the main focus on citizen health, mobility, active lifestyle, and well-being. The Laboratory is acting in the segment named Electronic Mobile Health (EMZ),



Figure 3: Prof. dr. Mihael Mohorčič and dr. Dušan Gabrijelčič presented successful Horizon 2020 energy research projects of the Jožef Stefan Institute in the European Parliament

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 the corresponding ICT platforms. The main contribution is in the development of methods and algorithms for securing the privacy of personal health data for all users of EMZ services. Security solutions are providing k-anonymity, l-diversity, and LKC-privacy. The research project titled **"Technological and business aspects of future ecosystem for e-health"** is focused on implementing the work within the priority area of the European cohesion policy "Smart cities

within the priority area of the European cohesion policy "Smart cities and communities". Its fundamental goal is the creation of a functional model to ensure sustainable technological and business development of an ecosystem for e-health. In 2018 we investigated how e-health platforms and applications could improve the hospital patient-discharge process.

Under the Infrastructure program in research organizations we keep providing support services that enable better communication 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 and for the emerging digital market. In 2018 the R&D activities in this field were focused on the research of novel security mechanisms and methods that enable the effective fight against cybercrime.

The fight against cybercrime was the main focus of the "Strengthening European Network Centres of Excellence in Cybercrime (SENTER)" project. SENTER has created a single point of reference for EU national cybercrime centres of excellence (CoE) and developed further national CoE into a well-defined and well-functioning community. The Laboratory for Open Systems and Networks was acting in the project as the Slovenian CoE. The project finished its activities in 2018 by formally establishing a non-profit association in Austria that will further facilitate cooperation between the centres of excellence and contribute to the domain of the fight against cybercrime.

The Laboratory for Open Systems and Networks is coordinating the "Criminal Justice Access to Digital Evidences in the Cloud - LIVE\_FORensics (LIVE\_FOR)" project from the EU DG Justice programme. The partners in this project 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 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 investigates the implementation of Directive 2014/41/EU, raises the awareness of the prosecutors and investigators of the new European tool for collecting cross-border evidence in the connected European digital world, establishes a collection of best practices, and develops standard educational content for train-

ing and education in the area of digital forensics. In 2018, the Laboratory members focused their work in LIVE\_FOR on the creation of educational services for judges, prosecutors and members of law-enforcement bodies, as well as on the research of the new European legal instruments, such as the proposed regulation on production and preservation orders. Prof.

## Our research and development results enable a more secure information society.

Borka Jerman Blažič received a plaque of appreciation at the HackIstanbul 2018 conference, where she presented the new legal instruments for cross-border crime investigation in the EU.

The research of the cross-border digital evidence collection and analysis of the Directive 2014/41/EU will continue in the new EU DG Justice programme project EIO-LAPD (European Investigation Order – legal analysis and practical dilemmas of international cooperation) where we will collaborate with six other institutions from Austria, Croatia, Germany, Italy, Slovenia and Portugal. The project will start in 2019.

Mathematical models for the construction of symmetric cryptographic algorithms were also the subject of research. Two methods have been developed. The first method enables infinite constructions of quadratic vectorial bent functions, which can be used as combinatorial objects with several areas of application. The results were published in the IEEE Transactions on Information Technology journal. The second method enables infinite constructions of semi-bent functions, which play an important role in the construction of orthogonal variable spreading codes used in code-division multiple-access (CDMA). The results were published in Information Processing Letters.

#### Internet services and applications

The main focus of the research and development 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 was to support and facilitate the learning process of PES (Public Employment

Services) practitioners in their professional identity development. The project partners have developed a set of services combining and linking eCoaching, reflection, MOOCs, networking, and analytical and learning support tools, leading to improved individual and organisational performance in the delivery of employment services. Privacy issues were also 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. The activities of the Laboratory members ensured that the tools developed were privacy aware, abided by privacy principles, and were compliant to the newest EU privacy and data-protection legislation.

The overall goal of the "Gameplay for Inspiring Digital Adoption (GIRDA)" project 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 investigate with field experiments the efficacy of an alternative approach to facilitating digital literacy and digital adoption based on digital games designed on touch-table technology devices.

The objective of the 3-year H2020 project "From Research to Policy through Raising Awareness of the State of the Art on Social Media and Convergence (COMPACT)" (October 2017-2020) is to increase awareness (including scientific, political, cultural, legal, economic and technical areas) of the latest technological discoveries among key stakeholders in the context of social media and convergence. The project is performing extensive research on policies and regulatory frameworks, as well as pre-standardization efforts in social media for preventing fake news, hate speech, and information disorder in general. The Laboratory for Open Systems and Networks leads the work package for policies and regulatory frameworks, where a methodology for examining the regulatory landscape across the EU countries has been developed and piloted. In 2018, the methodology was designed and piloted in 11 EU countries (Slovenia, Slovakia, Bulgaria, Greece, Croatia, Belgium, UK, Ireland, Latvia, Denmark and Portugal) in 75 organizations (fact-checking platforms, privacy initiatives, media-awareness initiatives, digital rights and gender civil groups, etc.). The results were analysed in the light of the current regulation and directives (GDPR, AVMSD, e-Commerce, etc.) from the aspects of addressing fundamental rights and regulatory implications (transparency and accountability). Based on the results, a reference



*Figure 4: Book about the Internet's arrival in Slovenia* 

#### Prof. Borka Jerman Blažič had a book published on the development and history of computer networks.

framework for information disorder was developed and a set of recommendations was extracted, based on which policy papers were developed. Next, the methodology will be implemented into the remaining EU countries and selected non-EU countries and a complete set of recommendations will be proposed for each relevant stakeholder according to the criteria investigated by the methodology.

#### 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.
- 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.], 2017, vol. 26, iss. 4, pp. 404-421.
- Pott, Alexander, Pašalić, Enes, Muratović-Ribić, Amela, Bajrić, Samed. On the maximum number of bent components of vectorial functions. IEEE transactions on information theory, ISSN 0018-9448, Jan. 2018, vol. 64, no. 1, pp. 403-411.

#### Awards and Appointments

- Prof. dr. Borka Jerman Blažič received recognition from The Program Committee of the Multiconference Information Society 2018 for the life work: "The First Lady of the Slovenian Internet", Ljubljana, October 12, 2018
- 2. Prof. dr. Borka Jerman Blažič received a recognition award at the "Hack Istanbul 2018" conference, Istanbul, Turkey, September 21–23, 2018.

#### Organization of conferences, congresses and meetings

1. Organization of the visit and seminar for members of the Posavje Society of Senior Managers and Experts, Jožef Stefan Institute, Ljubljana, Slovenia, April 13, 2018

## INTERNATIONAL PROJECTS

- 7FP EmployID; Scalable Cost-effective Facilitation of Professional Identity Transformation in Public Employment Services Asst. Prof. Tomaž Klobučar
- European Commission
- SENTER Strengthening European Network Centres of Excellence in Cybercrime Prof. Borka Džonova Jerman Blažič European Commission
- ERASMUS+; GIRDA Gameplay for Inspiring Digital Adoption Prof. Borka Džonova Jerman Blažič European Commission
- INEA/CEF eID4U; eID for University Asst. Prof. Tomaž Klobučar
- Innovation And Networks Executive Agency (inea) 5. LIVE\_FOR; Criminal Justice Access to Digital Evidences in the Cloud - LIVE\_FORensics
- Prof. Borka Džonova Jerman Blažič European Commission 6 INFA/CFF, SL-PASS Slovanian eIDAS Node and Integrated Ser
- INEA/CEF SI-PASS; Slovenian eIDAS Node and Integrated Services Asst. Prof. Tomaž Klobučar Innovation And Networks Executive Agency (inea)
- H2020 Flex4Grid; Prosumer Flexibility Services for Smart Grid Management Dr. Dušan Gabrijelčič European Commission
- H2020 DEFENDER; Defending the European Energy Infrastructures

## STAFF

- Researchers
- 1. Asst. Prof. Rok Bojanc\*
- 2. Prof. Borka Džonova Jerman Blažič, Head, until 31.03.18
- 3. Dr. Dušan Gabrijelčič
- 4. Asst. Prof. Tomaž Klobučar, Head, since 01.04.18
- Postdoctoral associates 5. Dr. Samed Bairić
- Dr. Samed Bajric
   Dr. Andrej Jerman Blažič
- Dr. Andrej Jerman Blazić
   Dr. Tanja Pavleska
- 8. Dr. Živa Stepančič

Dr. Dušan Gabrijelčič European Commission

 H2020 - COMPACT; From Research to Policy through raising Awareness of the State of the Art on Social Media and Convergence
 Dr. Tanja Pavleska
 European Commission

### **RESEARCH PROGRAM**

 Future Internet Technologies: concepts, architectures, services and socio-economic issues Prof. Borka Džonova Jerman Blažič

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

- 1. Smart City Ecosystem EkoSmart
- Dr. Živa Stepančič Ministry of Education, Science and Sport
- Strategic Research & Innovation Partnership (SRIP) Smart Cities and Communities Dr. Dušan Gabrijelčič
- Ministry of Economic Development and Technology 3. Technological and business aspects of future ekosystem for e-health Dr. Samed Bajrić
  - Ministry of Education, Science and Sport
- Dr. Marina Trkman Postgraduate
   Primož Cigoj, B. Sc. Technical officers
   Danijel Grah, B. Sc.
   Tatjana Martun, B. Sc.

Note: \* part-time JSI member

## BIBLIOGRAPHY

#### **ORIGINAL ARTICLE**

- Marina Trkman, Peter Trkman, "A framework for increasing business value from social media", *Ekonomska istraživanja*, 2018, **31**, 1, 1091-1110.
- 2. Alexander Pott, Enes Pašalić, Amela Muratović-Ribić, Samed Bajrić, "On the maximum number of bent components of vectorial functions", *IEEE transactions on information theory*, 2018, **64**, 1, 403-411.
- Živa Stepančič, Borka Jerman-Blažič, "Exploring European digital single market: user adoption and preferences for eID services", *International journal of electronic governance*, 2018, **10**, 4, 382-422.
- Andrej Jerman Blažič, Borka Jerman-Blažič, "Digital skills for elderly people: a learning experiment in four European countries", *Review of European studies*, 2018, **10**, 4, 74-86.

#### PUBLISHED CONFERENCE CONTRIBUTION

- 1. Martin Mihajlov, Borka Jerman-Blažič, "Eye tracking graphical passwords", In: Denise Nicholson (ed.), Advances in human factors in cybersecurity: proceedings of the AHFE 2017 International Conference on Human Factors in Cybersecurity, July 17-21, 2017, Los Angeles, California, USA, (Advances in intelligent systems and computing **593**), 2018, 37-44.
- Darinka Arh Pilih, Rok Bojanc, "Uvedba enotnega evropskega standarda za e-Račune v Sloveniji - ukrep ROSE", In: Špela Urh Popovič (ed.), Digitalizacija in mi: zbornik, 2018, 1-10.
- Živa Stepančič, Andrej Krpič, Kristjan Koželj, Damjan Bobek, Arso Savanović, Dušan Gabrijelčič, "Prosumer flexibility management in smart grids", In: Karolj Skala (ed.), MIPRO 2018: 41st International Convention, May 21 -25, 2018, Opatija, Croatia: proceedings, 2018, 479-484.
- 4. Borka Jerman-Blažič, Primož Cigoj, Andrej Jerman Blažič, "Learning digital skils for elderly people by using touch screen technology and

learning games: a case study", In: Bruce M. McLaren (ed.), *Proceedings* of the 10th International Conference on Computer Supported Education, 15-17 March, 2018, Funchal, Madeira, Portugal, (Science and Technology Publications 1), 2018, 222-229.

- 5. Massimiliano Massi, Tanja Pavleska, Helder Aranha, "Automating smart grid solution architecture design", In: *Proceedings of the 2018 IEEE International Conference on Communications, Control, and Computing Technologies for Smart Grids (SmartGridComm): 29-31 October 2018 in Aalborg, Denmark, 2018.*
- Samed Bajrić, "Can we trust cryptographers?", In: Tomi Mlinar (ed.), Nikolaj Simič(ed.), *Trusted internet: proceedings*, Štiriintrideseta delavnica o telekomunikacijah VITEL, 14. in 15. maja 2018, Brdo pri Kranju, Slovenija, 2018, 63-66.
- 7. Tanja Pavleska, "The causal loop between information disorder and trust on the Internet", In: Tomi Mlinar (ed.), Nikolaj Simič(ed.), *Trusted internet: proceedings*, Štiriintrideseta delavnica o telekomunikacijah VITEL, 14. in 15. maja 2018, Brdo pri Kranju, Slovenija, 2018, 57-66.

#### SCIENTIFIC MONOGRAPH

1. Borka Jerman-Blažič, Don Kihotka na Slovenskem ali Kako je internet prišel v Slovenijo: internet in Slovenija: 25 letna perspektiva, Ljubljana: eBesede: Institut Jožef Stefan, 2018.

#### ENCYCLOPAEDIA, DICTIONARY, LEXICON, MANUAL,

#### Atlas, Map

- 1. Dušan Zupančič, Alan Ružič, Rok Bojanc, Tomaž Močnik, Jorgo Bertalanič, Rok Bojkovič, *E-SLOG 2.0 Electronic invoice: English version*, [Ljubljana]: Gospodarska zbornica Slovenije, 2018.
- Dušan Zupančič, Alan Ružič, Rok Bojanc, Tomaž Močnik, Jorgo Bertalanič, Rok Bojkovič, *E-SLOG 2.0 elektronski račun: slovenska* različica, [Ljubljana]: Gospodarska zbornica Slovenije, 2018.

## DEPARTMENT OF COMMUNICATION E-6 **SYSTEMS**

The core activities of the Department of Communication Systems comprise the research, development and design of next-generation telecommunication networks, technologies and services; wireless communication, embedded and sensor systems; and new procedures and algorithms for parallel and distributed computing. Within these activities our research work includes the development of the methods and software tools for the modelling, simulation, analysis and synthesis of communication systems, pilots and experimental testbeds, 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 2018 the research activities within the Communication Technology Laboratory were concentrated on the Prof. Mihael Mohorčič challenges associated with the access-segment of radio technologies. We focused on the research of radio transmission in terrestrial and satellite communications and management of the radio and network resources. This research is a part of the research program on Communication networks and services (P2-0016).

The research on radio-signal propagation was directed in two main research areas, namely, the development of propagation channel models for frequency bands foreseen for future communication systems and the development of software tools for the simulation of radio-wave propagation. The first topic mainly concerns the research on high-speed train communications in the millimetre-wave (mmWave) frequency band. We studied the impact of typical railway objects on the mmWave propagation channel for intrawagon and train-to-infrastructure communications. Propagation measurements are conducted in the mmWave band for the 12 most common railway materials. The corresponding electromagnetic parameters are obtained, and a 3D ray-tracing simulator is calibrated. We are

also continuing the research of the geometry-based multipath model for a 3GPP mmWave high-speed train scenario. A full parameterization of the proposed model has been made. Since the measurement of the mmWave channel is deficient for the high-speed train scenario, we proposed a channel model using a ray-tracing simulator that is validated with the channel measurements performed in the high-speed train scenario at 93.2 GHz. The proposed geometrical method has been verified through a comparison of the proposed model results and the measurement-validated ray-tracing simulations in terms of the power delay profile, the Ricean K-factor, and the second-order statistics for the delay and angle domains.

The indoor radio ray-tracing method was revisited from the algorithmic point of view with the aim to use it for the characterization of dynamic radio environments, while the outdoor propagation modelling was upgraded by network optimization with a multi-objective evolutionary algorithm.

The second topic looked at the development, implementation and testing of a software tool for radio-wave propagation modelling and wireless communication networks' optimization. The tool is integrated into an open-source geographical information system (GIS) and incorporates statistical channel models and channel models based on ray-tracing and optimization procedures. We studied computationally efficient radio ray-tracing techniques in the context of physical channel models. The developed procedures were evaluated in the design and management of telecommunication networks. We looked at the design and implementation of a graphical user interface to make the tool user friendly and usable for the wider community.

Ray-tracing algorithms supported by many-core architectures and based on the brute-force approach have been studied extensively in indoor and outdoor environments. The far superior modelling of electromagnetic propagation effects than any other stochastic modelling is computationally demanding and requires extensive algorithmic optimization. In particular, detecting unique wavefronts at the observation point proves to be resource consuming because the geometry of the ray distribution in space does not allow a perfect detection of exactly one ray per wavefront, with the refraction and diffraction phenomena generating further irregularities.

In 2018 we were finalizing joint efforts with Xlab and Alanta to develop and launch the first cloud-based radiofrequency ray-tracing engine. The service will allow the wider incorporation of deterministic channel characterization in emerging communication systems even when dedicated computing resources on the required scale cannot



be provided on-site. The activities have a supporting role in the research of indoor localization techniques within the Communications Technology Laboratory.

The software tool for radio-wave propagation modelling in mobile communication systems and wireless communication systems optimization was upgraded by network optimization with a multi-objective evolutionary algorithm, which determines for a given set of criteria functions, the optimal network parameters. We added new criteria functions to also take into account the quality of the user experience. The basic criteria functions applied in the past, such as the network efficiency, reduce the necessary resources and consequently reduce the operational costs. Based on the terrain profile maps and construction locations, the tool calculates the path loss by applying

We incorporated findings, obtained during the previous studies of the thermal rating of a power transmission network, into the DiTeR software package that successfully passed testing and was selected for operational use in the Slovenian transmission network. state-of-the-art statistical models and determines the optimal allocation of users to the base-stations or base-station locations and their parameters by maximizing specified 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 for user based

of Slovenia that is operating in the VHF frequency band.

In this year we also concluded the H2020 project eWine "elastic WIreless Networking Experimentation". We continued 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, we upgraded the localization software toolbox with advanced cooperative localization methods.

In the field of wireless mesh networks, we continued to investigate network-coding techniques and networkcoding-aware routing procedures in order to increase the network capacity. We have designed a novel opportunistic network-coding procedure, which significantly improves the performance of different networks and supported applications in terms of throughput, delay and jitter. The proposed procedure was upgraded with a self-adaptive algorithm, which gives even better results. We have shown that opportunistic network coding can significantly improve the performance of different wireless networks and applications, in particular, if the usage of opportunistic network coding is considered upfront in the wireless network's design phase. We also presented a testbed for the evaluation of the network-coding-assisted retransmission scheme for multimedia broadcasting in wireless networks.



Figure 1: Visualization of the indoor signal power in the developed radio-frequency ray-tracing tool

In 2018 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 in the Ka-band (19.7 GHz) and the Q-band (39.4 GHz) beacon signals from the Alphasat satellite. The motivation behind the international activities is to collect as much of the propagation data and their mutual analyses as possible, and thus enable an in-depth research of the atmosphere's impacts on the satellite radio waves' propagation. In this respect we conducted statistical analyses of the fade duration and the fade slope of joint attenuation in the three-site satellite diversity experiment in Slovenia. The analyses are made on two-year collected measurements and also include single-site and two-site combinations. The analysis revealed that satellite site diversity significantly reduces the number of fades and the total fade times compared to a single-site link. The obtained results will enable engineers to develop efficient telecommunication technology for high satellite communication throughputs, achieving speeds of the order of up to Terabit/s. Within the project we started the collaboration with the HITEC Luxembourg S.A. company, for which we are, in addition to satellite signal, also collecting the time-dependent azimuth and elevation of the satellite antenna.

In 2018 we continued with active participation in the COST Action 15104 IRACON "Inclusive radio communication networks for 5G and beyond", where we are contributing to disciplinary working groups concerned with radio channel, physical layer and network layer, as well as to experimental working groups on localization and tracking and on the Internet of Things.

Research activities in the field of network optimization and management have also been applied to the field of smart grids. Their complexity is constantly increasing with the introduction of distributed electric generators and the introduction of electric cars, which in the near future will represent large electrical energy consumers and temporal energy storages. Therefore, the precise monitoring of the distribution network's status is the first prerequisite for the quality management of the grid. Thus, we focused on the development of a three-phase distribution system state

estimation with special attention being paid to state estimators that exhibit a robustness and insensitivity to bad data present in the input set of measurements. Based on the algorithms for numerical computation, the proposed solutions were evaluated on the reference IEEE distribution feeder.

In the **Parallel and Distributed Systems Laboratory**, we successfully continued interdisciplinary research work in the framework of the research programme that also includes the Laboratory for Machine Intelligence from the Faculty of Electrical Engineering and the Laboratory of Algorithmics from the Faculty of Computer and Information Science, both from the University of Ljubljana. We also cooperated with researchers from industry and medicine, on research projects and with joint papers.

The research topics of the laboratory principally involve solving computationally intensive problems and problems for which the computation is distributed over heterogeneous computer architectures. To this end, our activities are based on developing algorithms needed in various fields, including numerical simulations, multi-criteria optimizations, analyses of large amounts of data, graph theory and computer vision. Through the development of new parallel and distributed algorithms, and their use, we expect to move the limits of the solvable or the comput-

able, while also transferring the knowledge to the industry, for real-life applications. Namely, our scientific curiosity is also driven by real-world problems and it is our inherent goal to fuse the advances in computer science with the other fields of science that we will be engaged in during the implementation of applied projects.

In the year 2018 we successfully continued our work on the FWO project "Multi-Analysis of Fretting Fatigue Using Physical and Virtual Experiments". In the project consortium we cooperate with researchers from the University of Gent and the University of Luxembourg. Our task is to design and implement parallel programs for the accurate simulation of fretting cracks' propagation. We developed a program for the simulation of contact and conceived its parallelization.

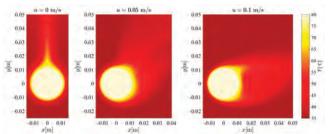


Figure 2: Temperature field in the vicinity of the transmission line at 0 m/s, 0.5 m/s and 0.1 m/s wind speeds.

In cooperation with the Milan Vidmar Electric Power Research Institute, for our client ELES, we finished the project "Cooling of Overhead Lines at Horizontal Speeds below 0.6 m/s". The findings were integrated into a physical model for the thermal rating of power lines, incorporated into the DiTeR software package. The main challenges in developing DiTeR were to achieve the real-time responsiveness of calculations, for the entire power system, and to achieve high reliability. DiTeR successfully passed the testing in a test environment and was selected in the tender of the Slovenian transmission operator for operative software implementing dynamic thermal rating of the Slovenian transmission network. In 2019, DiTeR is expected to become operational. Furthermore, it is part of the solution chosen at the tender of the Croatian power transmission system operator for the installation of a pilot system for monitoring the thermal conditions of their network. In the context of smart grids we also studied the impact of the uncertainty of the model and measurements on the network state estimation.

Together with an industrial partner, we continued the development of a system for continuous long-term ECG recording during daily activity, to the extent that our system is produced and successfully marketed under the Savvy trademark. Our ECG measuring device is a small and autonomous device for the unobtrusive long-term (weekly, monthly and longer) recording of the ECG activity. Measurements are wirelessly transmitted to a personal terminal, e.g., a smartphone, and, if necessary, a computer cloud. Devices such as this will form the basis of the

future tele-health services, which are essential for reducing the costs of general health care. Our ultimate goal is to monitor the ECG of thousands of users in the home environment and in real time. The cooperation is continued under a contract on the maintenance and further development of software and hardware.

We continued the project EkoSmart ("Ecosystem of a Smart City") from the Ministry of Education, Science and Sport, in the framework of the call for "RDI in chains and networks of values". Within the project we support

the implementation of pilot studies of the use of a mobile ECG recorder in a medical environment. We are exploring effective ways of analysing data and integrating them into the existing medical databases. In 2018 we started with the related H2020 project "Supporting Active Ageing through Multimodal Coaching (SAAM)". In SAAM, we provide body ECG sensors with a software environment that we are upgrading towards a system for unobtrusive monitoring of the elderly at home. A comprehensive description of our research in the field of body sensors and electrocardiography, from the aspect of wireless and mobile ECG monitoring, has been provided in our book Body Sensors and Electrocardiography, published by Springer in 2018. In the framework of the bilateral OTKA project "Graph Optimization and Big Data", financed by the Slovenian and the Hungarian research agencies, we addressed the Big Data challenge interpreted in terms of graph models and their processing. The project aims to prove theo-

In several projects we investigate complementary challenges for the use of 5G mobile networks for the provision of massive ultra-reliable low-latency communications for control, management and fault localization in smart energy grids. rems about model parameters, to design efficient parallel algorithms for model analysis and to implement these algorithms on the next-generation supercomputers. The research will contribute results relevant to graph theory and broader to discrete mathematics, as well as algorithms and methods useful for the more efficient processing of big data. The partnership on the project spurred ideas for further work, which will be continued on future joint projects. To this end, we are currently compiling a COST Action proposal. Within the COST Action IC1405 "Reversible Computation - Extending Horizons of Computing", we investigated conditions for the realizability and reversibility of global choreographies for systems with asynchronous inter-process communication. We have discovered the insufficiency of the conditions that were so far considered sufficient, and corrected them.

In the Networked Embedded Systems Laboratory we continued the research, design, development and implementation of advanced hardware and software solutions for connecting various things and devices with the aim to improve their accessibility, utility and efficiency. To this end we are making use of contemporary concepts



Figure 3: We co-organized the EuCNC 2018 conference on 5G and the Next Generation Internet technologies, services and applications with more than 500 attendees from around the world

such as service-oriented architecture, dynamic service composition, cognitive communications, Internet of Things and others. 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 also in 2018 the modular platform VESNA used for the development of wireless sensor networks. We further enhanced and upgraded the LGTC hardware module and corresponding software to support edge gateway functionality, edge computing, remote reconfiguration and remote debugging on devices with restricted capabilities. This module was used for the upgrade of the LOG-a-TEC wireless sensor network testbed at the premises of the Jožef Stefan Institute, which is part of the Next Generation Internet Experimentation (NGI-EXP) initiative (previously FIRE/ FIRE+ initiative) through the H2020 Fed4FIRE+ (Federation for FIRE plus) project and available through a common Fed4FIRE portal also to the community of external experimenters. The LOGa-TEC testbed was also upgraded with further communication modules supporting LoRa and IEEE 802.15.4 UWB technologies to support the investigation of performance optimization and the increase of the density of low-power wide area (LPWA) devices and localization in complex indoor environments.

In 2018 we continued with the research work in the H2020 projects eWINE, NRG-5, DEFENDER and SAAM, and we acquired a new basic research project funded by the Slovenian Research Agency J2-9232 "Resource management for low latency reliable communications in smart grids - LoLaG".

In eWINE, which was also successfully concluded in 2018, we continued the work on modelling the effects of indoor environments on localization with ultra-wideband (UWB) radio signals. By using convolutional neural networks, we developed models for the detection of non-line-ofsight (NLOS) propagation conditions and for ranging error estimation and thus significantly

improved the indoor localization algorithm accuracy. We continued the development of the machine-learning-based link quality predictor for the wireless link quality estimation (LQE) and novel approaches for sensing the radio spectrum occupancy and classification of detected radio technology.

We continued the investigation on link quality estimation and radio spectrum occupancy in the frame of the NRG-5 project, with the main emphasis being on the provision of massive ultra-reliable, low-latency communications for the control and fault localization in energy grids. We also participated in the development of a phasor measurement unit (PMU) and smart meter functions virtualization. These functions will be experimentally verified in the distributed laboratory environment, followed by pilot verification in a real operating environment.

The above research activities are complemented with basic research in the LoLag project (ARRS J2-9232), where we investigate the provision of ultra-reliable massive low-latency communications and edge computing to support real-time monitoring, autonomous protection and distributed control. In 2018 we started the project with the definition of representative wide-area monitoring system (WAMS) use cases for power-system operation and the specification of the corresponding requirements for communication interfaces.

In DEFENDER we continued with the design and implementation of advanced data-processing algorithms for the detection, identification and localization of cyber-physical threats based on data from PMU devices deployed in the energy grid. We started with a thorough experimental verification of those algorithms in a laboratory environment using a real-time digital simulation (RTDS) framework with hardware in the loop. After the verification the PMU devices will be deployed in a real operating pilot environment at the Italian Distribution System Operator ASM Terni for the demonstration of identification and the localization of cyber-physical threats.

In SAAM we designed the system architecture for unobtrusive sensing support for monitoring and identifying the activity of the elderly population in their home environment. We started with the adaptation of the existing VESNA sensing and communication modules and algorithms to enable multimodal activity and context monitoring via the energy consumption of home appliances and interference in the UWB radio channel. We also adapted the

LGTC module to support edge computing and gateway functionalities as well as to enable the remote configuration and management of connected devices. We implemented the required communication interfaces and protocols, and designed a remote monitoring and control platform. These activities will be followed by the testing and verification of individual system components, their integration and pilot validation in real home environments.

In June 2018 we co-organized in Ljubljana an international conference EuCNC 2018 (European Conference on Networks and Communications), which is an important recognition of our research work in the area of wireless and mobile communications. EuCNC is one of the biggest annual European events focusing on 5G and the Next Generation Internet technologies, services and applications. Last year it gathered more than 500 attendees from all over the world and was supported financially and in content also by the European Commission through the H2020 project EuCoNneCts3.

#### Some outstanding publications in the past year

- Kuhar, Urban, Pantoš, Miloš, Kosec, Gregor, Švigelj, Aleš. The impact of model and measurement uncertainties on a state estimation in three-phase distribution networks. IEEE transactions on smart grid, ISSN 1949-3053. [Print ed.], 2018, vol., no., str. 1-10, ilustr. https://ieeexplore.ieee.org/document/8331939/, doi: 10.1109/TSG.2018.2823398.
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#### Organization of Conferences, Congresses and Meetings

- 1. Meeting and worshop of the project H2020 SAAM, Ljubljana, 17 January 2018
- 2. Meeting of the FWO Lead Agency project G018916N "Multi-analysis of fretting fatigue using physical and virtual experiments", Ljubljana, 5–9 February 2018
- 3. European Conference on Networks and Communications EuCNC 2018, Ljubljana, 18-21 June 2018
- 4. Project final review H2020 "eWine", Ljubljana, 21-22 June 2018

#### Patent granted

 Branko Jenko, Gregor Kosec, Hrvoje Petković, Ajda Podgoršek Berke, Jerca Pahor, Alen Čusak, Oda Cornelia Maria Sibon, Balaji Srinivasan, Stable pantetheine derivatives for the treatment of pantothenate kinase associated neurodegeneration (PKAN) and methods for the synthesis of such compounds, US9963472 (B2), US Patent and Trademark Office, 08. 05. 2018.

## INTERNATIONAL PROJECTS

- COST IC1405; Reversible Computation Extending Horizons of Computing 1. Prof. Monika Kapus Kolar Cost Office
- COST IC1305; Network for Sustainable Ultrascale Computing (NESUS) 2 Prof. Roman Trobec
- Cost Office
- COST CA15104; Inclusive Radio Communication Networks for 5G and Beyond (IRACON) 3. Prof. Tomaž Javornik Cost Office
- ESA SatProSi-Alpha; Ka/Q-band Propagation Measurements and Modelling Slovenian 4. Contribution to the Alphasat TDP#5 Scientific Mission Dr. Andrei Vilhar
- Esa/estec.
- H2020 eWINE; Elastic Wireless Networking Experimentation 5. Prof. Mihael Mohorčič European Commission
- H2020 Fed4FIREplus; Federation for FIRE Plus 6. Prof. Mihael Mohorčič
- European Commission
- H2020 DEFENDER; Defending the European Energy Infrastructures 7. Prof. Mihael Mohorčič European Commission
- H2020 EuConNeCts3; European Conferences on Networks and Communications 8 (EuCNC)
- Prof. Mihael Mohorčič
- European Commission H2020 NRG-5; Enabling Smart Energy as a Service via 5G Mobile Network Advances 9 Dr. Carolina Fortuna
- European Commission 10. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching Prof. Mihael Mohorčič European Commission

## RESEARCH PROGRAMS

- Communication networks and services Prof. Mihael Mohorčič
- 2 Parallel and Distributed Systems Prof. Roman Trobec

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

- Graph Optimisation and Big Data 1. Dr. Matjaž Depolli
- 2 Multi-analysis of fretting fatigue using physical and virtual experiments Prof. Roman Trobec
- 3 Resource management for low latency reliable communications in smart grids - LoLaG Prof. Mihael Mohorčič
- 4 Advanced Ray-Tracing Techniques in Radio Environment Characterization and Radio Localization
- Prof. Mihael Mohorčič 5. Smart City Ecosystem - EkoSmart
- Prof. Roman Trobec
- Ministry of Education, Science and Sport
- Strategic Research & Innovation Partnership (SRIP) Smart Cities and Communities 6 Prof Mihael Mohorčič
- Ministry of Economic Development and Technology 7. Antenna Tracking System Simulator Verification Dr. Andrej Vilhar

Hitec Luxembourg S.a.

### NEW CONTRACTS

- The European Conference on Networks and Communications 2018 Prof. Mihael Mohorčič
- Cankarjev Dom 2. DTR software: DiTeR
- Dr. Gregor Kosec Eles, d. o. o.

## VISITORS FROM ABROAD

- Andreas Roepert, Interactive Wear AG, Starnberg, Germany, 17 January 2018 1 Claus Pribbernow, Interactive Wear AG, Starnberg, Germany, 17 January 2018, 2.
- 17-19 April 2018 Prof. Stéphane P. A. Bordas, Université du Luxembourg, Luxemburg, Luxemburg, 3. Cardiff University, Cardiff, Great Britain, 5-9 February 2018
- Prof. ir. Magd Abdel Wahab, Ghent University, Gent, Belgium, 5-9 February 2018 4
- Kyvia de Fatima Resende Pereira, Ghent University, Gent, Belgium, 5-9 February 2018 5.
- Dr Nermin Suljanović, Universitet u Tuzli, Bosnia & Herzegovina, 5 April 2018 6.
- Prof. Luis M. Correia, Instituto Superior Técnico, University of Lisbon, Lisbon, Portugal, 7 24 April 2018
- 8. Prof. Ke Guan, Beijing Jiaotong University, Beijing, China, 21 June 2018
- Luiz DaSilva, Trinity College Dublin, Ireland, 22 June 2018 9
- 10. Ingrid Moerman, imec, Leuven, Belgium, 22 June 2018
- Jorge Pereira, European Commission, Brussels, Belgium 22 May 2018 11.
- Ivan Boshkov, Ss. Cyril and Methodius University, Skopje, Macedonia, 1st October to 12 31st of December 2018
- 13. Rares Andrei Mosoi, Technical University of Cluj-Napoca, Romania, 2-8 December 2018

## **STAFF**

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- Dr. Viktor Avbeli 1.
- Dr. Matjaž Depolli 2
- Dr. Carolina Fortuna 3.
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- Prof. Monika Kapus Kolar 6.
- Dr. Gregor Kosec
- 8
- Prof. Andrej Lipej Prof. Mihael Mohorčič, Head 0
- 10. Asst. Prof. Roman Novak
- 11. Dr. Igor Ozimek
- 12. Dr. Aleksandra Rashkovska Koceva
- 13. Prof. Aleš Švigelj
- 14. Prof. Roman Trobec
- 15. Dr. Andrej Vilhar, left 15.10.18

#### Postgraduates

16. Klemen Bregar, B. Sc.

- Gregor Cerar, B. Sc.
   Jure Slak, B. Sc.
- Technical officers
- 19. Polona Anžur, B. Sc.
- 20 Miha Mohorčič B Sc 21. Miha Smolnikar, B. Sc.
- 22. Denis Sodin, B. Sc.
- Technical and administrative staff
- 23. Tomaž Krištofelc
- 24. Tamara Matevc, B. Sc.
- 25. Marko Mihelin\*, B. Sc.
- 26. Tomaž Šolc, B. Sc., left 01.07.18
- 27. Matevž Vučnik, B. Sc.

Note: \* part-time JSI member

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#### LECTURE)

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### INDEPENDENT COMPONENT PART OR A CHAPTER IN A

#### MONOGRAPH

- 1. Aleksandra Rashkovska, Roman Trobec, Viktor Avbelj, Matjaž Veselko, "Efficacy of cryotherapy for pain control after anterior cruciate ligament reconstruction", In: Chadwick C. Prodromos (ed.), *The anterior cruciate ligament: reconstruction and basic science*, 2018, 207-210.
- 2. Aleš Švigelj, Melisa Junuzović, "Network coding-assisted retransmission scheme for video-streaming services over wireless access networks", In: Abdelfatteh Haidine (ed.), Abdelhak Aqqal (ed.), *Broadband communications networks: recent advances and lessons from practice*, 2018, 123-142.
- Kemal Alič, Aleš Švigelj, "Opportunistic network coding", In: Marcus Greferath (ed.), *Network coding and subspace designs*, (Signals and Communication Technology) 2018, 319-338.

#### SCIENTIFIC MONOGRAPH

- 1. Roman Trobec, Ivan Tomašić, Aleksandra Rashkovska, Matjaž Depolli, Viktor Avbelj, *Body sensors and electrocardiography*, Cham: Springer, (Springer Briefs in applied sciences and technology), 2018.
- 2. Roman Trobec, Boštjan Slivnik, Patricio Bulić, Borut Robič, *Introduction to parallel computing: from algorithms to programming on state-of-the-art platforms*, Cham: Springer, (Undergraduate topics in computer science) 2018.

#### PATENT

1. Branko Jenko, Gregor Kosec, Hrvoje Petković, Ajda Podgoršek Berke, Jerca Pahor, Alen Čusak, Oda Cornelia Maria Sibon, Balaji Srinivasan, Stable pantetheine derivatives for the treatment of pantothenate kinase associated neurodegeneration (PKAN) and methods for the synthesis of such compounds, US9963472 (B2), US Patent and Trademark Office, 08. 05. 2018.

#### MENTORING

1. Urban Kuhar, *Three-phase state estimation in power distribution systems:* doctoral dissertation, Ljubljana, 2018 (mentor Aleš Švigelj; comentor Gregor Kosec).

# 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 non-deterministic systems. Our research results are implemented within applications for production, transport, energy, 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 2018 in the fields of efficient algorithms for massive-data processing, computing structures for the faster and more reliable execution of algorithms, and interactive interfaces for the efficient acquisition and handling of data were complemented by the design, development and implementation of various solutions within 13 European projects in *Horizon 2020, ECSEL/ARTEMIS, FP7, Interreg, COST* and *EFSA* programs, as well as in seven national projects.



Prof. Gregor Papa

#### Algorithms for Data Processing

The research in the field of efficient algorithms for data processing was focused on the development of multi-objective optimization approaches, approaches for statistical comparison and knowledge extraction, neural networks and pattern recognition. Several solutions were used on the application level within computer support for our *Open platform for clinical nutrition - OPEN* (http://www.opkp.si), as well as for intelligent support of smart factories and smart cities.

#### Optimization algorithms

In the field of **multi-objective optimization**, **supported by parallelization and surrogate modelling**, we continued with a Twinning project Horizon 2020 *SYNERGY* - *Synergy for smart multi-objective optimisation* (http://synergy-twinning.eu/). As part of the activities within the project we co-organized and participated in several events. During the event of the *Chamber of Commerce and Industry of Slovenia* in July we presented aspects of

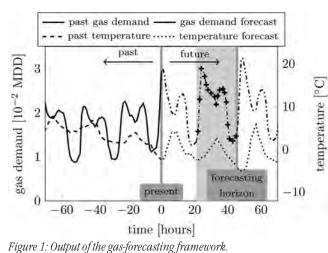
artificial intelligence in the context of smart factories. We outlined the main features and advantages of using artificial intelligence. On the example of the SYNERGY project, we presented our collaboration with Slovenian companies. In particular, we highlighted the optimization of production process parameters, optimal product design (technical and economic) and

## Optimization and uncertainty quantification are important factors in engineering design.

product quality control. These lead towards the implementation of artificial intelligence for use in digital twins. In May we co-organised the *International Conference on Bioinspired Optimization Methods and their Applications BIOMA 2018* in Paris, France. We received 69 submissions and based on the review process 27 long papers were accepted by authors from 18 countries. Papers were published in the Lecture Notes in Computer Science (LNCS) proceedings by Springer. In August we co-organized the *SYNERGY Summer School on Efficient Multi-Objective Optimisation* in Ljubljana, Slovenia. Three renowned researchers (prof. Enrique Alba, prof. Jürgen Branke, and prof. Carlos A. Coello Coello) presented their invited lectures, in addition to speakers from the SYNERGY project team (Peter Korošec, Bogdan Filipič, Boris Naujoks, and Nouredine Melab). The main goal of the summer school was to improve the awareness of multi-objective optimisation, parallelisation, surrogate modelling, and the synergy of all three research fields among the attendees. There were 47 attendants from 21 countries. To further promote the science and technology, the SYNERGY project supported a round table on *Women in Science and Technology* in December. Through five panellists and 46 attendees it discussed several open issues and suggested solutions to improve the careers of female researchers.

We continued with the Horizon 2020 Marie Skłodowska-Curie Actions project *UTOPIAE - Uncertainty Treatment and OPtimisation In Aerospace Engineering* (http://utopiae.eu/). The main aim is in bridging **optimization and uncertainty quantification** in aerospace systems applications. Developing fundamental mathematical methods and algorithms to bridge the gap between uncertainty quantification and optimization and between probability theory and imprecise probability theory for uncertainty quantification will lead to efficient solutions of high-dimensional, expensive and complex engineering problems. We hosted two researchers of the network, from *University of Strathclyde* and *ESTECO*, on their three-months secondment at our department, where they improved their knowledge on selected aspects of optimization.

The main objective of the ARRS research project *Biomedical data fusion by nonnegative matrix tri-factorization*, in collaboration with the *University of Ljubljana* is the development of new, efficient and accurate **methods for non-negative matrix factorization** required for analysing real-world, complex biomedical data. Several optimization algorithms for non-negative, tri-factorization problems of large matrices were developed. These include three gradient-based local search techniques, several configurations of single- and multi-objective evolutionary



algorithms and a hybrid algorithm that employs both evolutionary and local search techniques. A practical method for the orthogonality satisfaction of solutions was developed that works with all the mentioned optimization algorithms. Using this orthogonalization method the problem of nonnegative matrix factorization becomes equivalent to *k*-means clustering. Therefore, the proposed algorithms have a wide range of uses. The initial results were presented at the *International Conference on Metaheuristics and Nature Inspired Computing META 2018*.

We extended the research on the **simultaneous broadcasting of multiple messages** from the same source vertex in synchronous networks. This is considered under the restrictions that each vertex receives at most one message in a unit time step, every received message can be sent out only in the next time step, no message is sent to already informed vertices. The number of outgoing messages is unrestricted, messages have unit length, and we assume full-duplex mode. We developed a concept of level-disjoint partitions to study simultaneous broadcasting under this model. In this work we consider the optimal number of level-disjoint partitions. We also

provide a necessary condition in terms of eccentricity and girth on the existence of more v-rooted level-disjoint partitions of optimal height. In particular, we provide a structural characterization of the graphs admitting two level-disjoint partitions with the same root. The work was published in the *Applied mathematics and computa-tion* journal.

In cooperation with the *Department of Intelligent Systems* at the JSI and the *Faculty of Electrical Engineering* and Computer Science, University of Maribor, we organized, for the fifteenth consecutive year, the Nature-inspired algorithms workshop dealing with stochastic optimization techniques.

#### Statistical approaches

At the end of January, Tome Eftimov successfully defended his PhD thesis entitled *Statistical data analysis and natural language processing for nutrition science*. The work presented in the thesis is a synergy of statistics and natural language processing. He proposes an approach to explore a given domain. The part of statistics is focused on how to obtain more robust statistical results that need to be published, and the part of natural language processing is focused on the extraction and normalization of relevant scientifically published information in order to follow the new knowledge of the domain.

We presented an invited lecture at the *International Conference on Informatics and Information Technologies*, in Mavrovo, Macedonia. The lecture was related to a novel approach for statistical comparison, known as **Deep Statistical Comparison**, which provides more robust statistical results than previous state-of-the-art approaches when results are affected by outliers or statistically insignificant difference that could exist between data values. The work related to Deep Statistical Comparison was also an invited lecture at the *Faculty of Electrical Engineering and Information Technologies*, at the *Faculty of Computer Science and Engineering, Ss. Cyril and Methodius University*, Skopje, and at the *University of Salzburg*, Austria. The tutorial on proper statistical analysis was performed at the *International Joint Conference on Computational Intelligence IJCCI 2018*, Seville, Spain.

A paper on a data-driven preference-based approach that is a combination of multiple criteria decision analysis with deep statistical rankings was presented at the *International Conference on Bioinspired Optimization Methods and their Applications BIOMA 2018*. The work on Deep Statistical Comparison was also presented at the *Genetic and Evolutionary Computation Conference GECCO 2018*, in Kyoto, Japan.

As part of the *FP7* project *Era-Chair ISO-FOOD – ERA Chair for isotope techniques in food quality, safety and traceability* (http://isofood.eu) and the Horizon 2020 project *RICHFIELDS – Research Infrastructure on Consumer Health and Food Intake for Escience with Linked Data Sharing* (http://www.richfields.eu/), we worked on computer-based methodologies that can be used for automated dietary assessment. We performed a study that tested the combination of an established and a validated food-choice research method (the 'fake-food buffet') with a new food-matching technology to automate the data collection and analysis. The methodology combines fake-food image recognition using deep learning and food matching and standardization based on natural language processing. Food matching firstly describes each of the recognized food items in the image and then matches the food items with their compositional data, considering both their food names and their descriptors. The final accuracy of the deep-learning model trained on fake-food images acquired by 124 study participants and providing

fifty-five food classes was 92.18 %, while the food matching was performed with a classification accuracy of 93 %. These findings are a step towards automating dietary assessment and food-choice research. The methodology outperforms other approaches in pixel accuracy, and since it is the

## Deep Statistical Comparison provides more robust statistical results when affected by outliers.

first automatic solution for recognizing the images of fake foods, the results could be used as a baseline for possible future studies. As the approach enables a semi-automatic description of recognized food items (e.g., with respect to the EFSA FoodEx2 system), these can be linked to any food-composition database that applies the same classification and description system. This work was done in a collaboration with the *ETH Zürich*, Switzerland and *The University of Newcastle*, Callaghan, Australia. The results were published in the *Public Health Nutrition* journal.

Within the work performed in the FP6 *EuroDISH* project, we identified requirements for computer-supported food matching, in order to address not only national and European but also international current related needs. The work was published in the *Nutrients* journal.

#### Knowledge extraction

As a part of the Horizon 2020 project *RICHFIELDS*, we worked on methodologies that can be used for food data harmonization and interoperability. The work was presented in two conference papers at the *Knowledge Engineering and Ontology Development 2018* and the *Knowledge Discovery and Information Retrieval 2018*, Seville, Spain. In the first paper we presented an ontology-learning process using personalized dietary web services that are dealing with food-related data and knowledge rules. The second paper presented i) a methodology for a food ontology to which foods are linked, ii) a part that explains how the relevant foods can be extracted and represented in a structured way, and iii) a similarity measure that is used to link the foods to the ontology.

As a part of the ERA-Chair *ISO-FOOD* project, we published a joint work with the *Department of Environmental Sciences* at the Jožef Stefan Institute in the *Food Chemistry* journal. The work describes **linking and harmonizing different knowledge repositories** with respect to isotopic data. We propose an ISO-FOOD ontology as a domain

ontology for describing isotopic data within Food Science. The ISO-FOOD ontology consists of metadata and provenance data that needs to be stored together with data elements in order to describe isotopic measurements with all the necessary information required for future analysis. The work on the semi-automatic approach for borrowing missing nutrient values in food-composition databases was presented at the *Jožef Stefan International Postgraduate School conference*, and at the *EuroFIR Food Forum 2018*.

#### Neural networks

In the area of **pattern recognition**, we developed several **models for forecasting the natural-gas consumption** of an urban area using machine-learning and data-mining methods. By using historical gas-consumption data for Ljubljana, different forecast models for residential natural-gas demand were implemented and compared. The models forecast gas demand with hourly resolution up to 60 hours into the future. The model forecasts are based on past temperatures, forecasted temperatures and time variables, which include markers for holidays and other occasional events. Machine-learning models were considered, such as linear regression, kernel machine and artificial neural network. Additionally, empirical models were developed based on data analysis. The two most accurate models were found to be recurrent neural network and linear regression model. In a realistic setting such trained models can be used in conjunction with a weather-forecasting service to generate forecasts for future gas demand. The work was published in the *Energy* journal.

Further, we developed a **methodology for using a deep neural network** as an extremely fast heuristic for optimization problems. This methodology was applied to the protein-structure optimization problem. Deep neural networks were constructed that are able to partially solve a protein-structure optimization problem. The networks were trained using a reinforcement learning approach so that no experimental protein data is required, only evaluations of the protein's free energy. This means that training data is generated by simulation and not by using expensive experimental methods such as X-ray crystallography, NMR spectroscopy and electron microscopy. This methodology can be applied to other classes of optimization problems and

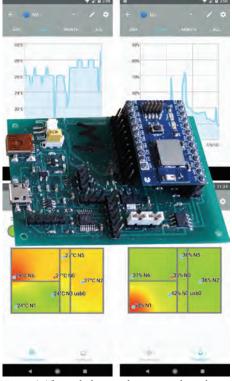


Figure 2: The multi-hop mechanism evaluated on a prototype board and its mobile monitoring platform.

represents a step towards an automatic heuristic construction using deep neural networks. Trained networks can be used to construct better initial populations for optimization. It was shown that differential evolution applied to a protein structure optimization problem converges to better solutions when the initial population is constructed in this way. The work was presented at the *International Conference on Bioinspired Optimization Methods and their Applications BIOMA 2018*.

In the area of **computer vision** within the project for the *International table tennis federation ITTF*, we developed a protocol for recording and automatic offline measurements of the table-tennis ball's height above the net and its speed in laboratory conditions. The protocol includes aligning the high-speed camera with the net, calibrating

#### A multi-hop communication mechanism makes it possible to acquire sensor data over an ad-hoc BLE sensor network.

it using the chessboard pattern, and then recording the game at a rate of 1000 fps, followed by the offline video processing. The developed protocol was used to record players of different skills at five different net heights in order to reach two objectives: to establish the impact of the net height on a table-tennis game and to investigate the correlation between the player's

skills and both measured parameters (ball speed, ball height). Five additional characteristic parameters (net errors, net balls, lets, net serve errors and average playing time) were statistically compared across the net heights to find out possible significant differences. While the results showed a strong correlation between the player's skills and both measured parameters the performed experiments did not show any significant influence of the net height on the table-tennis game. The project activities and the conclusions were presented at the *World Congress of Racket Sport Science* in Bangkok, Thailand.

#### Databases

We collaborate with the research group at the Milko Kos Historical Institute of the *Research Centre of the Slovenian Academy of Sciences and Arts* on the project "Slovenia Historical Topography". Historical topography of the territory of the Republic of Slovenia has been a desideratum of Slovenian historical science for almost a century. The goal of the project will be to produce a thorough and reliable interactive digital version of the historical topography of the entire territory of the present-day Republic of Slovenia. The first part, which covered the territory of the historical province of Carniola, has already been successfully achieved. The resulting web page is available at http://topografija.zrc-sazu.si/. The second part is a historical topography of the Slovene Littoral (Primorska region). The research is financially supported by the *Slovenian Research Agency* and the *Slovenian Academy of Sciences and Arts*.

#### **Computing Structures**

To support and accelerate our algorithms several approaches were studied and developed on the level of hardware and computing structures, which includes the use and **online reconfiguration of FPGAs**, customized embedded systems and sensors.

We developed an FPGA implementation of a systolic array for matrix multiplication using fixed-point arithmetic for the acceleration of the deep learning of neural networks. An accelerator is integrated with our PCI-E prototyping platform to achieve high data throughput. Acceleration with stand-alone (embedded) systems using network communication for data exchange is studied to compare with the integrated solution. The work was presented at the *International Conference on Microelectronics, Devices and Materials MIDEM 2018* in Ljubljana.

In the field of **embedded systems**, we developed a Bluetooth low-energy multi-hop communication mechanism that enables acquiring sensor data over an ad-hoc BLE sensor network. The BLE 4.0 protocol supports only the Piconet topology and does not support data transfer over multiple nodes. To overcome this limitation a mechanism to relay sensor data over multiple BLE 4.0 nodes using Master/Slave switching was developed. The mechanism dynamically creates communication paths within the BLE ad-hoc sensor network of identical BLE nodes. Using this mechanism, the range of the sensor data's acquisition can be extended from the BLE range to the whole BLE sensor network. The multi-hop mechanism was evaluated on a prototype board and is described in a paper published in *Informacije MIDEM* journal.

The multi-hop mechanism was further upgraded to support different sets of sensor data and extended with an error-recovery mechanism. An updated mechanism was used in a mobile monitoring platform that consists of a BLE sensor network, data-acquisition system, web service system, and mobile application. The platform was presented at the *International Conference on Microelectronics, Devices and Materials MIDEM 2018* and in a graduate thesis at the *Faculty of Computer and Information Science, University of Ljubljana*.

One of the objectives of the Horizon 2020 *RICHFIELDS* project was to develop a method for estimating food portions. For this aim, we improved our kitchen scales that was originally developed for FIT diabetic patients who need to calculate insulin bolus considering the content of carbs in the meal. The scale was enhanced with a BLE 4

communication module, weight measurement bridge, and high-precision AD converter. The scale operating time was maximized by powering down the peripheral devices while the scale is not used.

In the field of the **usage of mobile and wireless sensing for cognitive load inference** our research focus stems from the need to manage human attention, which, as evident by the competition among computing devices and services trying to attract a user, is the most precious resource in the information age. Our attention is limited, above all, by our cognitive capacities and multitasking capabilities. In this line of research, we investigated how mobile and wireless sensing can be harnessed to automatically infer a user's cognitive load, and consequently, adapt human-computer interaction so as to create a more efficient, task-relevant, and less stressful environment for the user. Our initial results on using wearables, such as smart wristbands equipped with heartbeat, skin conductance and similar sensors, to infer cognitive load were presented in October 2018 at *UbiTtention: International Workshop on Smart & Ambient Notification and Attention Management*. At the same workshop we presented our efforts

towards completely unobtrusive wireless sensing of a user's cognitive load based on wireless radar technology. Finally, our overview of attentionmanagement systems in ubiquitous computing, together with guidelines for future research in this area has been published by *Proceedings of the ACM on Interactive, Mobile, Wearable and Ubiquitous Technologies (IM-WUT)* and presented at the *ACM UbiComp 2018* conference in Singapore.

In the frame of Horizon 2020 *TETRAMAX - Technology Transfer via Multinational Application Experiments* (https://www.tetramax. eu/) project in the scope of the European "*Smart Anything Everywhere*" initiative in the domain of **customized low-energy computing** (CLEC) for cyber-physical systems and the internet of things, we organised two workshops. The first workshop was organized in cooperation with the *Center for Technology Transfer and Innovation*, as a part of the multi-conference "Creative international synergies, cooperation with industry and the use of online platforms". The second workshop addressed the companies that are looking for opportunities for access to the CLEC technologies to innovate their products and/or services. It was organized in cooperation with the *SRIP Factories of the Future*. Among the presentation of the open calls and the project ambitions, the representatives of two Slovenian companies, who obtained funding for implementation of their projects at the first TETRAMAX open call, shared their experiences with the participants.



Figure 3: Wi-Mind system uses a high-frequency radar to capture minute movements of a human body that correspond to breathing and heartbeat activity. These, in turn, can be linked with a user's cognitive load at the time of measurement.

#### Sensors

In the scope of sensors research we studied the ageing of LTCC-based (Low Temperature Co-fired Ceramic) pressure sensors under different operating conditions from the maintenance strategy point of view. We focused on changes in the sensor response due to the long-term operation in normal conditions and under the conditions of frequent overloading in different environments. Our experiments showed that both the intensity and frequency of the overloads can result in larger drifts of the sensor's response from the calibrated response and in the larger scattering of the measurement results. Frequently, in the water and wet environments overloading reduces the lifetime of the LTCC sensors more than overloading in the air. In addition, possible intrinsic defects, non-detected by typical testing in serial production, may further shorten the sensor lifetime under the operation with frequent overloads. These results and the measures proposed can be considered more generally for sensor technologies and can serve as guidelines for implementing maintenance strategies.

#### Human-Computer Interaction

In the area of efficient interaction systems, we focused on the study of **usage scenarios** within a human-machine interaction, usability testing, as well as the development of **serious games for tele-rehabilitation**, and web tools for nutrition and food informatics.

Within the ECSEL project *MANTIS* – *Cyber Physical System based Proactive Collaborative Maintenance* (http://www.mantis-project.eu/), we contributed to the **HMI framework for system maintenance**. The developed HMI model allows us to conceive the HMI framework for a given use case and to define its particular content elements, their functionalities and input/output data at the desired level of detail, both at the early design phase and during implementation. The framework can also serve other purposes, for example, to identify content elements involved in context-awareness issues and provide the basis for analysing developed solutions. In scope of this we designed the presentations for some use-case scenarios. We presented the way how context-aware based alarms could be used in railway maintenance with color-coded animated indicators placed on the map.

Gregor Papa co-edited *The MANTIS book*, which highlights the fundamentals of Condition-Based Maintenance related conceptual ideas, an overall idea of preventive maintenance, the economic impact and technical solution, as outcomes of the MANTIS project. The core content of the book describes the creation of a maintenance-oriented reference architecture that supports the maintenance data lifecycle, to enable the use of novel kinds of maintenance strategies for industrial machinery. The key enablers are collecting data through Cyber-Physical Systems, the usage of machine-learning techniques and advanced visualization for the enhanced monitoring of the machines. This book is suitable for industrial and maintenance managers that want to implement a new strategy for maintenance in their companies.

We developed several **web tools for nutrition and food informatics**. Within the *FOOD LABELS* project, we collaborated with the *Administration of the Republic of Slovenia for Food Safety, Veterinary Sector and Plant Protection* and developed a web tool for calculating and checking the food label with respect to the EU Regulation on the provision of food information to consumers. The tool enables an easy calculation of the food label using national food composition data. Within the project *Innovative solutions for informed decisions* in collaboration with *NUTRIS - Inštitut za nutricionistiko* and *Zveza potrošnikov Slovenije* we are preparing a national database of branded foods and a **mobile application Veš**, **kaj ješ**.

In frame of the Horizon 2020 project REFRESH - Resource Efficient Food and dRink for the Entire Supply



Figure 4: MANTIS-based context-aware alarms to be used in railway maintenance with colour-coded animated indicators placed on the map.

#### Usability testing

*cHain* (http://eu-refresh.org/) we developed the **web tool FoodWasteEXplorer for gathering and handling of data of food waste** and developed web services to connect the web tool with other information systems. The application is aimed mainly at researchers and industrial partners performing the valorisation of food wastage and is available at https://ws.eurofir. org/FoodWasteExplorer/login.htm. Within the *REFRESH* project 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 have contributed to a national survey on dietary habits by developing a web tool for 24h recall that is primarily aimed at collecting food consumption data and submitting it to the *European Food Safety Agency*. As food consumption data needs to be linked with the food composition data to become valuable, we applied our method *StandFood* that enables quick and precise matching of food-consumption data with the corresponding food-composition data.

The goal of UsabEU is to provide a starting point for usability evaluations with questionnaires in the native or mother tongue. The platform supports the online collaborative translation of usability questionnaires and their validation. Additionally, it serves as a repository for all the validated questionnaires and as a tool to perform statistically sound usability evaluations. The current proof-of-concept platform supports the translation and validation of the System Usability Scale questionnaire and statistical assistance for sample size estimation and data summarization.

The importance of nutrition for Parkinson's disease patients has been acknowledged in many papers. On the other hand, the usability of tools supporting nutrition interventions is not well studied. This paper presents a case study on how to design a nutrition-tracking mobile application for users with Parkinson's disease. We focus on the design choices made to accommodate users and findings from usability testing with users. Both works will be presented at the *Human-Computer Interaction International 2019*.

#### Tele-rehabilitation

In the scope of Horizon 2020 project *PD\_manager – mhealth platform for Parkinson's disease management* (http://www.parkinson-manager.eu/), our objectives were to design intensive target-based physiotherapy for upper extremities suitable for tele-rehabilitation services and examine the clinical meaningfulness of the exergaming at an unchanged medication plan. A **tele-rehabilitation exergaming system** using the Kinect sensor was developed; 28 patients with PD participated in the study. The system followed the participants' movements and adapted the difficulty level of the game. The outcomes of the study showed that seven out of 26 participants could set up the equipment at home alone. Clinical outcomes of Box and Blocks Test, UPDRS III, and daily activity Jebsen's test; writing a letter; and moving light objects were statistically significant and considered clinically meaningful. The Nine-Hole Peg Test showed a statistically nonsignificant improvement. The findings lead to preliminary conclusions that exergaming is feasible, but may require technical assistance, whereas clinically meaningful results could be

achieved according to validated instruments and an unchanged medication plan in individuals with PD. The work was published in *International journal of rehabilitation research*.

#### User interfaces

In collaboration with partners and end-users, we analysed user needs and defined appropriate user experiences and designed corresponding interfaces for several tools related to nutrition.

School pot (http://solskilonec.si): to provide the planning of healthy meals in kindergartens, schools and dormitories. We created an interface that enables users to easily construct a daily menu and see if it fits the required nutritional guidelines for children of the specified age. This was achieved with dynamic visualizations of nutritional quantities that included the desired ranges of parameters taken from nutritional guidelines. We focused on making the visual information on each step as easy to process as possible (by using platform-wide colour-coding for each parameter, increased visual weight of indicators, uniform position of visualization on each page, etc.) and as a result reduced the cognitive load of users in their meal-planning tasks.

Bazil (http://bazil.si): to provide a platform for managing a food-composition database established at IJS in cooperation with the *Institute for nutrition* and the *Ministry of health*. We made it possible for administrators to quickly navigate the database records of nutrition projects by designing easy-to-manage filtering and sorting possibilities. We simplified the input of information from photographs of newly added products by designing an easy-to-switch system between input fields and photos. We established a clear visual hierarchy of search and product pages that enables users to quickly review and successfully find the required information from the vast quantity of nutrition data.

Food labels (https://prehranskeoznacbe.si): to provide support for food producers in food labelling in Slovenia. The designed interface allows users to input ingredients rapidly and is significantly reducing the required clicks in the process. We provided users with automatically-calculated nutritional results from their data by guiding them through the process in easy-to-follow steps. We enabled users to successfully manage their collection of products by displaying items in a structure that enables quick navigation and edits of their nutrition data.

FoodWasteEXplorer (https://ws.eurofir.org/foodwasteexplorer): for reducing food waste across the EU and maximizing the value from food waste and packaging materials. We proposed layout improvements that support users in finding the desired information when using the tool for reviewing food-waste data. The improvements focused on restructuring the sequence of required steps, establishing a clearer hierarchy of visual information and simplifying the input process of food names, categories and taxonomies.

Veš, kaj ješ (https://veskajjes.si/): to inform the public about healthy nutritional choices by visually communicating certain nutritional information. Since one of the project partners took a different approach, our interface design then was not included in the final product, but is nonetheless believed to teach important lessons to the team.

#### Some outstanding publications in the past year

- 1. Rok Hribar, Primož Potočnik, Jurij Šilc, Gregor Papa, "A comparison of models for forecasting the residential natural gas demand of an urban area", Energy, 167: 511-522, 2019, doi: 10.1016/j.energy.2018.10.175.
- 2. Petr Gregor, Riste Škrekovski, Vida Vukašinović, "Modelling simultaneous broadcasting by level-disjoint partitions", Applied mathematics and computation, 325: 15-23, 2018, doi: 10.1016/j.amc.2017.12.018.
- Marina Santo-Zarnik, Franc Novak, Gregor Papa, "Sensors in proactive maintenance: a case of LTCC pressure sensors", Maintenance and reliability, 20 (2): 267-272, 2018, doi: 10.17531/ein.2018.2.12.
- Tome Eftimov, Gordana Ispirova, Doris Potočnik, Nives Ogrinc, Barbara Koroušić-Seljak, "ISO-FOOD ontology: a formal representation of the knowledge within the domain of isotopes for food science", Food chemistry, 277: 382-390, 2018, doi: 10.1016/j.foodchem.2018.10.118.
- Imre Cikajlo, Alma Hukić, Irena Dolinšek, Dejana Zajc, Mateja Vesel, Tatjana Krizmanič, Bojan Blažica, Anton Biasizzo, Franc Novak, Karmen Peterlin-Potisk, "Can telerehabilitation games lead to functional improvement of upper extremities in individuals with Parkinson's disease?", International journal of rehabilitation research, 41 (3): 230-238, 2018, doi: 10.1097/MRR.000000000000291.
- 6. Barbara Koroušić-Seljak, Peter Korošec, Tome Eftimov, et al., "Identification of requirements for computersupported matching of food consumption data with food composition data", Nutrients, 10 (4): 433-450, 2018, doi: 10.3390/nu10040433.
- Simon Mezgec, Tome Eftimov, Tamara Bucher, Barbara Koroušić-Seljak, "Mixed deep learning and natural language processing method for fake-food image recognition and standardization to help automated dietary assessment", Public health nutrition, 1-10, 2018, doi: 10.1017/S1368980018000708.

#### Organization of conferences, congresses and meetings

1. 32nd Slovenian Workshop on Nature-Inspired Algorithms, Donačka mountain, 25. 5. 2018

- Workshop Tetramax "Creative international synergies, collaboration with industry and the use of online 2. platforms", Ljubljana, 15. 6. 2018
- 3. Summer School Synergy, Ljubljana, 27. 8. - 31. 8. 2018
- Workshop Tetramax "How to get a grant for your project on open TETRAMAX calls", Ljubljana, 12. 12. 2018 4.
- 33rd Slovenian Workshop on Nature-Inspired Algorithms, Ljubljana, 14. 12. 2018 5.

## INTERNATIONAL PROJECTS

- SYNERGY Summer School on Efficient Multi-Objecitve Optimisation, Ljubljana, 27.-1 31.8.2018
- Prof. Peter Korošec 2 EU MENU Slovenija; LOT 1; Support to National Dietary Survey in Compliance with the EU MENU Methodology - Fourth Support
- Prof. Barbara Koroušić Seljak
- European Food Safety Authority Efsa
- EU MENU Slovenija; LOT 2; Support to National Dietary Survey in Compliance with the 3. EU MENU Methodology - Fourth Support Prof. Barbara Koroušić Seljak
- European Food Safety Authority Efsa
- 4 COST CA15140 - ImAppNIO; Improving Applicability of Nature-Inspired Optimisation by Joing Theory and Practise Dr. Vida Vukašinović
  - Cost Office
- 5. H2020 - MANTIS; Cyber Physical System based Proactive Collaborative Maintenance Prof. Gregor Papa
- European Commission H2020 - REFRESH; Resource Efficient Food and Drink for the Entire Supply Chain 6.
- Prof. Barbara Koroušić Seljak European Commission
- 7. H2020 - RICHFIELDS; Research Infrastructure on Consumer Health and Food Intake using E-science with Linked Dara Sharing Prof. Barbara Koroušić Seljak
- European Commission
- H2020 eHERITAGE; Expanding the Research and Innovation Capacity in Cultural 8 Heritage Virtual Reality Applications
- Prof. Gregor Papa
- European Commission 9 H2020 - UTOPIAE; Uncertainty Treatment and OPtimization in Aerospace Engineering
- Prof. Gregor Papa European Commission
- H2020 TETRAMAX; TEchnology TRAnsfer via Multinational Application eXperiments 10 Dr. Marina Santo Zarnik
- European Commission 11. H2020 - SAAM; Supporting Active Ageing through Multimodal Coaching Prof. Barbara Koroušić Seljak European Commission
- 12. H2020 PD\_manager; Mhealth Platform for Parkinson's Disease Management Prof. Barbara Koroušić Seljak
- European Commission 13. H2020 - SYNERGY; Synergy for Smart Multi-Objective Optimisation Prof. Peter Korošec
- European Commission
- 7 FP; ERA CHAIR ISO-FOOD Era Chairs for Isotope Techniques in Food Quality, Safety 14. and Traceability Prof. Barbara Koroušić Seljak

European Commission

## VISITORS FROM ABROAD

- Prof. Sophia Ananiadou, University of Manchester, Manchester, Great Britain, 30. 1. -1. 31. 1. 2018
- Stefan Kochev, Faculty of Computer Science and Engineering, Ss Cyril and Methodius 2 University, Skopje, Macedonia, 20. 7. - 20. 9. 2018
- 3. Gorjan Popovski, Faculty of Computer Science and Engineering, Ss Cyril and Methodius University, Skopje, Macedonia, 20. 7. - 20. 9. 2018
- STAFF
- Researchers
- Asst. Prof. Anton Biasizzo 1
- Prof. Peter Korošec 2 3. Prof. Barbara Koroušić Seljak
- 4 Prof. Franc Novak
- 5. Prof. Gregor Papa, Head
- 6. Asst. Prof. Veljko Pejović\*

- RESEARCH PROGRAM
- 1. Computer Structures and Systems Prof. Gregor Papa

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

- Biomedical data fusion by nonnegative matrix tri-factorization
- Prof. Gregor Papa Advanced electrocaloric energy Conversion 2 Prof. Barbara Koroušić Seljak
- 3. Toponomastical heritage of Primorska Region Dr. Jurij Šilc
- Synergic Networking for Innovativeness Enhancement of central european actoRs 4 focused on hiGh-tech industry
- Prof. Gregor Papa Interreg Central Europe Programme
- Upgrade of the web portal for school nutrition "Šolski lonec" with respect to the national dietary guidelines Prof. Barbara Koroušić Seljak
- Ministry of Health
- Innovative solutions for informed food choices for healthier consumers Prof. Barbara Koroušić Seljak Ministry of Health
- Strategic Research & Innovation Partnership Factories of the Future (SRIP PMIS) Prof. Gregor Papa
- Ministry of Economic Development and Technology
- Upgrade of the Open Platform for Clinical Nutrition to suit the needs of the Federation 8 of EU member National Associations of Dietitians EFAD Prof. Barbara Koroušić Seliak
- Eurofir Aisbl iNet - The Impact of Net Height in Table Tennis 9 Dr. Drago Torkar
- International Table Tennis Federation

### NEW CONTRACTS

- 1. FOOD LABELS: Application of Food Labeling Prof. Barbara Koroušić Seljak Administration of the Republic of Slovenia for Food Safety, Veterinary Sector and Plant Protection
- 2 My Milk 2: 24 hour recall Prof. Barbara Koroušić Seljak University Medical Centre Ljubljana, Division of Paediatrics
- Monika Simjanoska, Faculty of Computer Science and Engineering, Ss Cyril and Methodius University, Skopje, Macedonia, 31. 7. 31. 8. 2018 4. 5
- Gianluca Filippi, University of Strathclyde, Glasgow, Scotland, 1. 9. 30. 11. 2018
- 6. Peter Zeno Korondi, ESTECO SpA, Trieste, Italy, 1. 9. - 30. 11. 2018
- Dr. Marina Santo Zarnik 8 Dr. Jurij Šilc 0 Dr. Drago Torkar Postdoctoral associates
- 10. Dr. Bojan Blažica
- 11. Dr. Tome Eftimov 12. Dr. Marko Pavlin\*

 Dr. Vida Vukašinović Postgraduates
 Margarita Antoniou, B. Sc.
 Rok Hribar, B. Sc.
 Gordana Ispirova, B. Sc.
 Urban Škvorc, B. Sc.
 Eva Valenčič, B. Sc.
 Technical officers Peter Novak, B. Sc.
 Špela Poklukar, B. Sc., left 01.05.18
 Technical and administrative staff
 Jolanda Jakofčič
 Andreja Vlašič, B. Sc.

Note: \* part-time JSI member

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## DEPARTMENT OF KNOWLEDGE **TECHNOLOGIES** E-8

The Department of Knowledge Technologies is involved in the development of artificial intelligence methods and advanced information technologies aimed at acquiring, storing and managing knowledge to be used in the development of the 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 develop applications in environmental sciences and management, agronomy, medicine, biomedicine and bioinformatics, economics, finance and marketing. The department is also a recognised centre of linguistic research and digital humanities.



In 2018 we were involved in sixteen national projects, ten Horizon 2020 projects, one COST action, one INTER-REG V-A Slovenia-Italy project, one infrastructure project, one smart specialization project, one bilateral project, and two industry projects. The department hosted seven junior researchers working towards their PhDs.

In the area of intelligent data analysis and data mining we developed several new methods and used them Prof. Nada Lavrač in a number of application domains. In the area of heterogeneous network analysis we developed a method for targeted end-to-end knowledge-graph decomposition. In the area of semantic data mining we developed a method for community-based semantic subgroup discovery. In the area of redescription mining, we have developed a new redescription mining method using a random forest of multi-target predictive clustering trees. In the area of applying data-mining methods in biology, we contributed to the discovery of dependencies between the domains of redox potential and plant defence through triplet extraction and copulas and a method for improving "bois noir" identification with interpretable black-box models. Within the H2020 project PD\_manager, which we coordinated, we developed a method for the analysis of medication change in Parkinson's disease progression, a method for detecting symptoms and medication change patterns for Parkinson's disease patients stratification, and a method for the visualization and analysis of Parkinson's disease status and therapy patterns. We successfully finalised the H2020 FET Innovation Launchpad project CF-Web that was aimed at investigating and establishing the means for

commercialization of the Web data-mining platform ClowdFlows. Within the SAAM H2020 project "Supporting Active Ageing through Multimodal Coaching", aimed at developing a Virtual Assistant-Coach that supports the aging population living at home, we have in 2018 developed the architecture of this coaching system. For the project F4F (Food 4 Future) we have designed a methodology for distinguishing between natural and synthetic aromas.

In the area of the automated modelling of dynamic systems, we have proposed a network reconstruction approach that relies on decoupling the approximation of network dynamics. Decoupling approximation consists of matching the simulated against the actual trajectories, for each node individually, rather than for the entire network at once. An important aspect of the proposed method is that it is relatively independent of the dynamical regime and the properties of the trajectories at hand. Moreover, the proposed method is extremely robust to both the length and resolution of the input trajectories and relatively insensitive to noise. Furthermore, we developed a visualization tool aiding the task of process-based modelling.

In the area of mining big and complex data, we developed various methods addressing different machine-learning tasks. First, we extended and designed novel methods for feature ranking in the context of structured output prediction. We proposed methods based on the Relief method and ensembles of trees for feature ranking for hierarchical multi-label classification as well as Relief for multi-label classification. Moreover, we proposed quantitative scoring functions for assessing the quality of feature rankings. Second, we proposed novel tree ensemble and rule ensemble

Marko Bohanec and coworkers organised an international conference IFIP DSS 2018, "The 19th Open Conference of the IFIP WG 8.3 on Decision Support Systems", which was held on June 13-15, 2018, at the Jožef Stefan Institute. More information: http://ifip2018dss.ijs.si/



Figure 1: A network of responses of the 565 lobby organizations to 21 public consultations in Banking and Finance. Two organizations are linked if they respond to the same consultation. Different colours denote the five detected communities. The communities are labelled by the prevailing topics in common consultations. The node size is proportional to the number of consultations to which the organization responded.

methods with random output selection for multi-target regression. Third, we developed methods for learning trees and ensembles of trees for semi-supervised, multi-target regression. Next, we investigated different approaches for structuring the output space in multi-label classification. Furthermore, we developed option predictive clustering trees for multi-label classification. In addition, we extended our semantic/ontological resources towards repositories of data-mining and machine-learning datasets, methods and experiments. Finally, we developed option predictive clustering trees for multi-target regression.

We have applied the developed methods to the analysis of data from life sciences and ecological modelling. Considering applications in the life sciences, we first developed and evaluated an in-silico framework for drug repositioning for tuberculosis and salmonella infections. Second, we performed a comprehensive evaluation of

Nada Lavrač had an invited lecture with the title "From relational to semantic data mining" at BIDAS - 3rd Bilbao Workshop on Data Science (Bilbao, Spain, 9. 11. 2018). the generalized relevance approach to inferring gene regulatory networks. Third, we showed that the evolutionary signal in metagenome phyletic profiles is useful for predicting gene functions. Next, we identified FREM2 and SPRY1 as new glioblastoma marker candidates using meta-analysis and experimental validation. Furthermore, we used semi-supervised classification trees to predict bacterial phenotypes. Concerning applications

in ecological modelling, we analysed the relationship between temperature and multi-proxy tree-ring records in climate reconstruction. In addition, we modelled the vessel lumen area tree-ring parameter of Quercus robur.

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. Two novel methods for mining redescription sets were developed: the first extends the redescription mining framework with random forests of predictive clustering trees and the second with multi-view learning.

In the area of **knowledge discovery from ecological and agriculture data** we were involved in several projects where we applied data-mining and decision-support methodologies for the development of predictive and decision-support models in the area of agronomy and systems ecology. In the H2020 project LANDMARK (Land Management, Assessment, Research, Knowledge base) we continued with the development of models for the prediction of soil functions. The results of these studies were published in a special issue of the Regional Environmental Change Journal. Prediction models for other soil functions were also developed and are in the process of validation with the domain experts. In addition, we used data mining for the prediction of N-mineralization in grassland soils

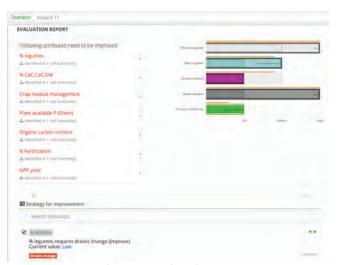


Figure 2: Screenshot of the user interface of the Soil Navigator decisionsupport system for assessment of the five soil functions, which also suggests measures to improve them.

in Ireland. An important part of our research activities in the LANDMARK project was the development of multiple attribute decision models using the DEX methodology for the assessment of five soil functions. For each soil function DEX model, validation and sensitivity analysis were performed. In the case of the primary productivity decision model, the calibration was made using data mining. The DEX methodology was also used to structure the farmers' and stakeholders' knowledge obtained at the 32 LANDMARK workshops. Two decision models were developed to evaluate the "knowledge" and "needs" of farmers regarding the soil functions. In the LANDMARK project we are also responsible for the development of a decision-support system Soil Navigator, which will be used for the assessment of soil functions, and we developed a user interface that enables communication between the user and the system. The user interface is in the process of testing and adjusting according to the users' needs.

The results of the research carried out in the concluded project EVADIFF "Evaluation of existing models and development of new decision-making tools to prevent diffuse pollution caused by phytopharmaceutical products" (2012–2015) on modelling the risk of pollution of water with pesticides were published in the journal "Environmental Science and pollution research international". A conference paper on predictive models for modelling drainage water outflow from agricultural fields was also published.

The final project results were presented at an invited talk at the 19th Open Conference of the IFIP WG 8.3. on Decision Support Systems, Ljubljana, Slovenia, where the developed decision-support system for the sustainable use of plant-protection products was presented. A large part of the activities in the BioDiv project were connected to the pre-processing of data about *Carabidae* species. The analyses of taxonomic and functional diversity indicated the presence of a large number of different carabid species in the Boigneville area (France). We constructed predictive models for the prediction of the abundance of the most abundant predator species. The results were presented to the wider scientific audience, who showed great interest in this work. In the H2020 project TRUE (TRansition paths to sUstainable legume based systems in Europe) we had two invited talks about sustainability indicators and their use in conceptual models for the assessment of the sustainability of legume agri-food chains. The identified sustainability indicators were used for the development of knowledge taxonomies, which will be later used for the development of a decision-support system for sustainability assessment. The current results were published in the journal "Impact". In the H2020 project TomRes, "A novel and integrated approach to increase multiple and combined stress tolerance in plants using tomato as a model" we organised a workshop to define the most suitable indicators for water and nutrient use efficiency in tomatoes. We also discussed the conditions and criteria that need to be taken into account for the development of a decision-support system for the management of the eco-physiological stress in tomatoes.

In the area of **text and web mining**, and heterogeneous information network analysis we successfully completed the H2020 FET project DOLFINS (Distributed Global Financial Systems for Society) and completed the work on a national project FORMICA (Influence of formal and informal corporate communications on capital markets). 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, annual reports, and other relevant data (stock prices, register of lobby organizations, public consultations etc.).

We proposed a methodology to properly evaluate Twitter sentiment (or stance) classification models for Twitter-specific time-ordered data. The classification models are constructed using text-mining methods, from a large set of manually annotated tweets by domain experts, and result in high-quality domain- and language-specific models. We showed that the standard cross-validation approach is appropriate to evaluate such models only if one applies blocked cross-validation, and does not randomly shuffle the examples. We analysed the properties of European lobby organizations from the Transparency Register, and from the open public consultations in the area of Banking and Finance. The 2008 financial crisis unveiled the intrinsic failures of the financial system as we know it. As a consequence, impact investing started to receive increasing attention, as evidenced by the high market-growth rates. The goal of impact investment is to generate social and positive environmental impact alongside a financial return. We used Twitter as a proxy of the impact investing market, and analysed relevant tweets posted over a period of 10 months. We identified the main players in the sector and how they interact and communicate with each

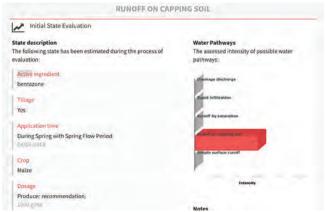


Figure 3: Screenshot of the user interface of the decision-support system for the environmentally friendly use of plant-protection products.

other. In the scope of the Formica project, we have developed methods for the analysis of financial texts, including the adaptation of a hybrid method for detecting semantic orientations, proposed novel methods for analysing diachronic changes of financial concepts in annual reports through the detection of lexical changes and the analysed expression of trust and doubt in tweets and reports.

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 2018, we published a paper in which we proposed methodological extensions of the qualitative multi-criteria modelling method DEX, as a basis for future long-term research and development in this area. In this context, we developed a novel algorithm, called jRule, for creating decision rules from DEX decision tables, which is substantially more efficient than the previous one. The year

2018 was the last year of two H2020 projects aimed at developing decisionsupport platforms and systems for severe chronic diseases: the Parkinson's disease (project PD\_manager) and congestive heart failure (HeartMan). In PD\_manager, we developed and evaluated decision-support models for suggesting medication change. In HeartMan, we developed models for the management of patients' physical exercises and contributed to the design of the clinical trial protocol. As a result of a previously completed EU project Co-Extra, we published results of a comparative analysis and evaluation

Sašo Džeroski had an invited lecture with the title "Mining big data and complex data" at the 24<sup>th</sup> International Symposium on Foundations of Intelligent Systems (ISMIS 2018), (Limasol, Cyprus, 29-31. 10. 2018)

of fifteen analytical methods for the detection of genetic organisms in food and feed. Our methods and tools were also successfully applied in the areas of evaluation of spatial design solutions, discovering dependencies between expert domains, selection of computer components and prediction of ski injuries.

In the area of **language technologies and digital humanities** we work on producing various types of language resources and on methods to annotate and analyse text, with a focus on the Slovenian and related languages.

In 2018 we concluded our work in the scope of the national research project JANES "Resources, Tools and Methods for Research of Non-standard Internet Slovenian". We edited a monograph that presented the results of the project,

e.g., the developed JANES corpus, tools to process non-standard Slovenian and the produced training datasets, as well as chapters on linguistic investigations that were made possible by the developed corpus and tools, e.g., on spelling practices in internet Slovenian, on (non)normativity of computer-mediated communication in Slovenian as regards the use of the comma, on tweets as a lexicographic source for the analysis of semantic shifts in Slovenian, on speech elements in non-standard internet Slovenian, and on code-switching in the posts of Slovenian Twitter users. In the last year of the project we also performed a number of other linguistic investigations connected with non-standard and internet Slovenian, in particular a discourse analysis of the Twitter campaigns connected to the referendum for the equalisation of same-sex marriages in Slovenia, an analysis of tweets of Slovenian corporate users, the attitude towards language in Slovenian, Croatian and Serbian computer-mediated communication, and a corpus analysis of non-standard use of the comma after introductory adverbial phrases. We also analysed collocations in computer-mediated communication from the perspective of lexicography. We were among the editors of the "Proceedings of the 6th Conference on Computer-Mediated Communication and Social Media Corpora" and gave an interview on internet Slovenian on the national radio. Various tools for the processing and analysis of Slovene computer-mediated content have been incorporated into the ClowdFlows platform for reusable workflows. We have developed methods for automated gender profiling, where classification models for five languages were also



athway ID Pathway description 3.001630 Prosphorylation 3.004648 Protein phospharylation 3.004429 Cellular protein metabolic process 3.001169 Tanumembrane receptor protein tyrosine kinase signaling pathwa 3.0018106 Peptidyl-tyrosine phosphorylation 3.003556 Intracellar signal franzoduction 3.003556 Cell surface receiptor signaling pathwaty 3.004237 Cellular metabolic process 3.004237 Cellular metabolic process 3.004237 Cellular metabolic process 3.004237 Cellular metabolic process

Figure 4: Identification of host (human) kinases controlling intracellular M. tuberculosis survival. The corresponding gene network is displayed along the top 10 enriched GO terms in the "Biological Function" category.

proposed as reusable workflows and were evaluated in various in-genre and cross-genre settings. We have analysed differences in language use between Slovene male and female bloggers. We have participated in the PAN shared task, where we proposed a deep-learning approach to multilingual gender classification from heterogeneous data sources, namely text and images.

We continued our research in the field of terminology, where we started a new basic research project TERMFRAME "Terminology and Knowledge Frames across Languages" in collaboration with the Faculty of Arts, University of Ljubljana. We also continued our work in the scope of the national research project KAS "Slovenian scientific texts: resources and description", where we produced two training sets for terminology extraction and investigated the derivational and inflectional characteristics of Slovenian scientific texts. We also worked on methods for automated

bilingual term alignment, started work on measures for readability assessment, and analysed collocations in the Slovene developmental corpus Šolar. We have also started developing methods for incorporating semantics into neural architectures.

We continued work on the national research project FRENK "Resources, methods, and tools for the understanding, identification, and classification of various forms of socially unacceptable discourse in the information society", where we worked on distributional modelling for semantic shift detection and on producing datasets of Slovenian and Croatian moderated news comments and organised and edited the proceedings of the 2nd Workshop on Abusive Language Online.

Thanks to the cooperation established in the already-concluded COST action ENeL, the European Network for Lexicography, we worked on predicting concreteness and imageability of words within and across languages via word embeddings and investigated semantic role labelling in Slovenian and Croatian.

We lead the Slovenian research infrastructure CLARIN.SI, which provides easy publication and sustainable access to digital language data for scholars in the humanities and social sciences. In 2018, 30 new resources were deposited in the CLARIN.SI repository, reaching 109 at the end of the year. A special mention is deserved by the second version of the SlovParl corpus, the Slovenian parliamentary debates from the period of secession, the Parlameter corpus of contemporary Slovenian parliamentary proceedings, hr500k, a reference training corpus of Croatian, and Opus-MontenegrinSubs, the first parallel English-Montenegrin electronic corpus. We also continued our work on the collaborative development of gold-standard resources for Slovenian, Croatian and Serbian. CLARIN.SI became one of the founding members of SLING, the Slovenian national supercomputer network, and supported the organisation of the EURALEX International Congress, which took place in Ljubljana in July. CLARIN.SI was one of the organisers of the "Conference on Language Technologies and Digital Humanities", which took place in Ljubljana in September 2018, and where we were among the Steering Committee members of the conference and the editors of the conference proceedings. We also investigated and presented various principles of Open Science, such as proper citation of language resources in Slovenian scientific publications and the use of FAIR principles in ethnography.

We were active not only nationally, but also in the European CLARIN ERIC, where we edited Volume 1 of "Tour de CLARIN" and presented CLARIN at several conferences, again, especially in connection with its role in enabling Open Science. We led the CLARIN's "Key resources families" initiative, where we covered second-language corpora and resources, corpora for parliamentary discourse research, spoken, historical, and parallel corpora, as well as

analysed usability issues of CLARIN's Virtual Language Observatory. Finally, we organised and edited the proceeding of the ParlaCLARIN workshop on creating and using parliamentary Corpora.

We contributed to the work of the Slovenian Institute for Standardization as the Slovenian representatives in ISO/TC37/SC4 (Terminology and Other Language and Content Resources / Language Resources Management) by reviewing, translating and approving Slovenian standards from this field. We also continued to serve as technical editors for the on-line Slovenian Biographical Lexicon, which we presented at the "Second Conference on Biographical Data in a Digital World".

In the area of **computational creativity**, we contributed an overview of the computational creativity field in Slovenia, analysed the historiography of the field based on the papers published in the "Proceedings of the International Conference on Computational Creativity", discussed the infrastructure for creative software blending, and proposed a system for automated slogan generation. Computational creativity methods and tools for bisociative knowledge discovery were presented at an invited talk.

#### Some outstanding publications in the past year

- 1. Mozetič, I., Torgo, L., Cerqueira, V., Smailović, J. How to evaluate sentiment classifiers for Twitter timeordered data?, PLoS ONE 13(3): e0194317, doi: https://dx.doi.org/10.1371/journal.pone.0194317, 2018.
- Bučar, J., Žnidaršič, M., Povh, J. Annotated news corpora and a lexicon for sentiment analysis in Slovene. Language resources and evaluation, ISSN 1574-020X, 2018, vol. 52, iss. 3, pp. 895-919, https://link.springer. com/article/10.1007/s10579-018-9413-3, doi: 10.1007/s10579-018-9413-3.
- Fišer, D., Ljubešić, N., Erjavec, T. The Janes project: language resources and tools for Slovene user generated content. Language resources and evaluation, ISSN 1574-020X, 2018, pp. 1-24, https://link.springer.com/ article/10.1007%2Fs10579-018-9425-z, doi: 10.1007/s10579-018-9425-z.
- Trajanov, A., Kuzmanovski, V., Réal, B., Marks P., Jonathan, Džeroski, S., Debeljak, M. Modeling the risk of water pollution by pesticides from imbalanced data. Environmental science and pollution research international, ISSN 0944-1344, 2018, vol. 25, no. 19, pp. 18781-18792, doi: 10.1007/s11356-018-2099-7.
- Levatić, J., Kocev, D., Ceci, M., Džeroski, S. Semi-supervised trees for multi-target regression. Information sciences, ISSN 0020-0255, 2018, vol. 450, pp. 109-127, doi: 10.1016/j.ins.2018.03.033.
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- Kralj, J. Robnik Šikonja, M., Lavrač, N. HINMINE : heterogeneous information network mining with information retrieval heuristics. *Journal of intelligent information systems*, ISSN 0925-9902, 2018, vol. 50, no. 1, pp. 29-61, doi: 10.1007/s10844-017-0444-9.

#### Awards and appointments

- 1. Matej Petković: Gold award at the Mathematical Competition "Kangaroo" 2017/2018, Ljubljana, Slovenia
- 2. Aneta Trajanov: Best Poster Presentation Award, Ljubljana, The 19th Open Conference of the IFIP WG 8.3 on Decision Support Systems, poster: "Validation of decision support models using data mining: a case study on primary productivity in agricultural fields in France"

#### Organization of conferences, congresses and meetings

- 1. The 2<sup>nd</sup> Human Brain Project Conference, Ljubljana, 14.–16. 2. 2018
- Project meeting HinLife, Analysis of heterogeneous information networks for knowledge discovery in life sciences, Kranjska Gora, 12.–14. 2. 2018
- "The 19th Open Conference of the IFIP WG 8.3 on Decision Support Systems (IFIP DSS 2018)", IJS, Ljubljana, 13.–15. 6. 2018
- 4. Project meeting H2020 EU project TOMRES "A novel and integrated approach to increase multiple and combined stress tolerance in plants using tomato as a model", City hotel Ljubljana, 21.–23. 3. 2018

- 5. Meeting of INTERREG V-A 2014-2020 project TRAIN, IJS, Ljubljana, 1. 2. 2018
- Project meeting H2020 EU project SAAM "Supporting Active Ageing through Multimodal coaching", Bled, Slovenia, 17.–19. 4. 2018
- "The Eleventh International Ljubljana-Zagreb Workshop on Knowledge Technologies", Dolenjske Toplice, 29.–31. 5. 2018

## INTERNATIONAL PROJECTS

- BIODIV Understanding and Managing Biodiversity in Agricultural Ecosystems by Data Mining and Decision Support
   Brof Sexo Decession
- Prof. Sašo Džeroski Arvalis - Institut Du Végétal
- COST CA16204; Distant Reading for European Literary History Prof. Tomaž Erjavec
- Cost Association Aisbl
- H2020 DOLFINS; Distributed Global FInancial Systems for Society Prof. Igor Mozetič European Commission
- H2020 HBP SGA1; Human Brain Project Specific Grant Agreement Prof. Sašo Džeroski
- European Commission
- H2020 TRUE; Transition Paths to Sustainable Legume based Systems in Europe Prof. Marko Debeljak European Commission
- H2020 TomRes; A Novel and Integrated Approach to increase Multiple and Combined Stress Tolerance in Plants Using Tomato as a Model Prof. Marko Debeljak
- European Commission
- H2020 LANDMARK; LAND Management: Assessment, Research, Knowledge Base Prof. Marko Debeljak European Commission
- H2020 NARSIS; New Approach to Reactor Safety Improvements Prof. Marko Bohanec
- European Commission 9 H2020 - SAAM: Supporting
- H2020 SAAM; Supporting Active Ageing through Multimodal Coaching Asst. Prof. Bernard Zenko European Commission
- H2020 HBP SGA2; Human Brain Project Specific Grant Agreement 2 Prof. Sašo Džeroski
- European Commission
- H2O20 PD\_manager; Mhealth Platform for Parkinson's Disease Management Dr. Dragana Miljković European Commission
- 12. H2020 HeartMan; Personal Decison Support System for Heart Failure Management Prof. Marko Bohanec
- European Commission 13. H2020 - CF-Web; ClowdFlows Data and Text Analytics Marketplace on the Web Asst. Prof. Martin Žnidaršič
- European Commission 14. Fellowship to visit ERC Grantee Asst. Prof. Vedrana Vidulin
- Slovenian Research Agency

## RESEARCH PROGRAM

1. Knowledge Technologies Prof. Nada Lavrač

- R & D GRANTS AND CONTRACTS
- Molecular bases of interactions among the grapevine and phytoplasmal causing agents of the grapevine yellows diseases Prof. Nada Lavrač
- Development of a multimethod approach to study wildlife behavior: investigating humanbear conflicts in contrasting landscapes of Europe Prof. Sašo Džeroski
- Influence of formal and informal corporate communications on capital markets Dr. Senia Pollak
- Collocation as a basis for language description: semantic and temporal perspectives Dr. Nikola Ljubešić
- 5. TermFrame: Terminology and Knowledge Frames across Languages
  - Dr. Senja Pollak Slovene scientific texts: resources
- Slovene scientific texts: resources and description Prof. Tomaž Erjavec
- Analysis of heterogeneous information networks for knowledge discovery in lifesciences
- Prof. Nada Lavrač
- Machine Learning for Systems Sciences Prof. Sašo Džeroski
- Resources, methods and tools for the understanding, identification and classification of various forms of socially unacceptable discourse in the information society Prof. Tomaž Erjavec
- 10. Semantic Data Mining for Linked Open Data Science Prof. Nada Lavrač
- 11. Improving Reproducibility of Experiments and Reusability of Research Outputs in Complex Data Analysis
- Asst. Prof. Panče Panov 12. Neuropsychological dysfunctions caused by low level exposure to selected environmental pollutants in susceptible population – NEURODYS Prof. Sašo Džeroski
- Forbidden Books in the Slovenian Lands in the Early Modern Period Prof. Tomaž Eriavec
- Structured output prediction with applications in sustainable agricultural production Prof. Sašo Džeroski
- 15. Food for future F4F
- Asst. Prof. Bernard Ženko
- Ministry of Education, Science and Sport 16. TRAIN: Big Data and Disease Models: A Cross-border Platform for Validated Biotech Industry Kits
  - Prof. Sašo Džeroski
- Regione Autonoma Friuli Venezia Giulia, Direzione
- 17. Data Mining and Decision support in Sustainable Food Production Dr. Vladimir Kuzmanovski
- Ministry of Education, Science and Sport 8. Learning models of diseases and treatments for systems and personalized medicine
- Dr. Jovan Tanevski Ministry of Education, Science and Sport 19. ReLDI - Regional Linguistic Data Initiative
- Dr. Nikola Ljubešić University Of Zurich, Urpp Language qnd Space
- The 19th Open Conference of the IFIP WG 8.3 on Decision Support Systems (IFIP DSS 2018), JSI, Ljubljana, Slovenia, 13 15 June 2018 Prof. Marko Bohanec
- Financing project visits at Slovenian higher education institutions Prof. Nada Lavrač Ministry of Health

## VISITORS FROM ABROAD

- 1. Prof. dr. Luis Torgo, Department of Computer Science, Faculty of Sciences, University of Porto, Porto, Porto, Portugal, 14.–19. 1 2018
- Claus Pribbernow, Interactive Wear AG, Starnberg, Germany, 16.–19. 1. 2018 and 18.–21. 9. 2018
- 3. Jihed Khiari, NEC Europe Ltd, Heidelberg, Germany, 29.-30. 1. 2018
- Dr. Matthew Purver, Queen Mary University of London, London, Great Britain, 27. 2.-1.
   3. 2018 and 12.-14. 3. 2018, 19.-20. 3. 2018, 20. 6. 2018
- Prof. dr. Donato Malerba, Università degli Studi di Bari "Aldo Moro", Bari, Italy, 13.–15.
   3. 2018
- Dr. Tony Veale, University College Dublin, Dublin, Ireland, 22.–27. 3. 2018
   Prof. dr. Albert Bifet, Laboratoire de Traitement et Communication de l'Information
- (LTCI), Télécom ParisTech, France, 28. 3.-4. 4. 2018
   Prof dr Hannu Toivonen University of Helsinki Helsinki Finland 25.-28. 4. 2018
- Prof. dr. Hannu Toivonen, University of Helsinki, Helsinki, Finland, 25.–28. 4. 2018
   Dr. Matej Mihelčić, Institut Rudjer Bošković, Zagreb, Croatia, 7–11. 5. 2018
- Annual Report 2018

- 10. Dr. Ivica Dimitrovski, Ss. Cyrill and Methodius, Faculty of Computer Science and Engineering, University of Skopje, Skopje, Macedonia, 17.-24. 6. 2018
- 11. Dr. Taru Sandén, Austrian Agency for Health and Food Safety (AGES), Vienna, Austria, 17.-18.7.2018
- 12. David Wall, Teagasc, Johnstown Castle, Co., Wexford, Ireland, 17.-18. 7. 2018
- 13. Dr. Michiel Rutgers, Centrum Duurzaamheid, Milieu en Gezondheid, Netherlands,
- 24.-27.7.2018
- 14. Dr. Van de Broek Marijn, ETH, Switzerland, 24.-27. 7. 2018
- 15. Prof. dr. Mateja Jamnik, Department of Computer Science and Technology, Computer Laboratory, University of Cambridge, Cambridge, Great Britain, 22. 8. 2018-5.8. 2019

#### STAFF

#### Researchers

- Prof. Marko Bohanec 1.
- Prof. Bojan Cestnik\*
- Prof. Marko Debeljak 3.
- Prof. Sašo Džeroski 4.
- Prof. Tomaž Erjavec 5.
- 6. Dr. Darja Fišer\*
- Dr. Dragi Kocev 7.
- Prof. Nada Lavrač. Head 8
- Prof. Zoran Levnajić\* 9.
- 10. Dr. Nikola Ljubešić
- 11. Prof. Igor Mozetič
- 12. Prof. Ljupčo Todorovski\*
- 13. Prof. Tanja Urbančič\*
   14. Asst. Prof. Vedrana Vidulin\*
- 15. Asst. Prof. Bernard Ženko
- 16. Asst. Prof. Martin Žnidaršič
- Postdoctoral associates
- 17. Dr. Božidara Cvetković
- 18. Dr. Jan Kralj
- 19. Asst. Prof. Petra Kralj Novak
- 20. Dr. Janez Kranjc
- 21. Dr. Vladimir Kuzmanovski
- 22. Asst. Prof. Biljana Mileva Boshkoska
- 23. Dr. Dragana Miljković 24. Dr. Blaž Mramor, left 01.10.18

## BIBLIOGRAPHY

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- 2. Tomaž Berčič, Marko Bohanec, Lučka Ažman Momirski, "Role of decision models in the evaluation of spatial design solutions", Annales: anali za istrske in mediteranske študije. Series historia et sociologia, 2018, 28, 3, 621-636.
- 3. Petra Kralj Novak, Luisa De Amicis, Igor Mozetič, "Impact investing market on Twitter: influential users and communities", Applied network science, 2018, 3, 40.
- 4. Borut Sluban, Mojca Mikac, Petra Kralj Novak, Stefano Battiston, Igor Mozetič, "Profiling the EU lobby organizations in banking and finance", Applied network science, 2018, 3, 44.
- 5. Anita Valmarska, Dragana Miljković, Spyros Konitsiotis, Dimitros Gatsios, Nada Lavrač, Marko Robnik Šikonja, "Symptoms and medications change patterns for Parkinson's disease patients stratification", Artificial intelligence in medicine, 2018, 91, 82-95.
- 6. Anneleen Baert, Els Clays, Larissa Bolliger, Delphine De Smedt, Mitja Luštrek, Aljoša Vodopija, Marko Bohanec, Paolo Emilio Puddu, Maria Constanza Ciancarelli, Michele Schiariti, Jan Derboven, Gennaro Tartarisco, Sofie Pardaens, on behalf of the HeartMan consortium, "A personal decision support system for heart failure management (HeartMan): study protocol of the HeartMan randomized controlled trial", BMC cardiovascular disorders, 2018, 18, 186.
- 7. Nejc Trdin, Marko Bohanec, "Extending the multi-criteria decision making method DEX with numeric attributes, value distributions and relational models", Central European Journal of Operations Research, 2018, 26, 1, 1-41.

- 16. Paolo Mignone, Università degli Studi di Bari "Aldo Moro", Bari, Italy, 27. 9. 2018 1. 2 2019
- 17. Dr. Serena Zacchigna, International Centre for Genetic Engineering and Biotechnology - ICGEB, Trieste, Italy, 18. 10. 2018
- 18. Dr. Nadja Ring, International Centre for Genetic Engineering and Biotechnology -ICGEB, Trieste, Italy, 18. 10. 2018
- 19. Dr. Simone Vodret, International Centre for Genetic Engineering and Biotechnology -ICGEB, Trieste, Italy, 18. 10. 2018
- 25. Dr. Aljaž Osojnik 26. Asst. Prof. Panče Panov 27. Dr. Vid Podpečan 28. Dr. Senja Pollak 29. Dr. Nikola Simidjievski 30. Dr. Jovan Tanevski 31. Dr. Aneta Trajanov 32. Dr. Anita Valmarska 33. Dr. Anže Vavpetič, left 15.01.18 Postgraduates 34 Martin Breskvar B Sc. 35. Matej Martinc\*, B. Sc. 36. Matej Petković, B. Sc. 37. Andraž Repar, B. Sc. 38. Tomaž Stepišnik, B. Sc. 39. Blaž Škrlj, B. Sc. 40. Tadej Škvorc, B. Sc. 41. Katja Zupan\*, B. Sc. Technical officer 42. Milica Bauer, B. Sc. 43. Nika Eržen, B. Sc Technical and administrative staff 44. Tina Anžič, B. Sc.

Note: \* part-time JSI member

- 8. Ivica Slavkov, Jana Karcheska, Dragi Kocev, Sašo Džeroski, "HMC-ReliefF: feature ranking for hierarchical multi-label classification", Computer science and information systems, 2018, 15, 1, 187-209.
- 9. Irma Ravkic, Martin Žnidaršič, jan Ramon, Jesse Davis, "Graph sampling with applications to estimating the number of pattern embeddings and the parameters of a statistical relational model", Data mining and knowledge discovery, 2018, 32, 4, 913-948.
- 10. Jernej Jevšenak, Tom Levanič, Sašo Džeroski, "Comparison of an optimal regression method for climate reconstruction with the compare\_methods() function from the dendroTools R package", Dendrochronologia, 2018, **52**, 96-104.
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- 12. Pavle Boškoski, Andrej Debenjak, Biljana Mileva Boshkoska, "Rayleigh copula for describing impedance data - with application to condition monitoring of proton exchange membrane fuel cells", European journal of operational research, 2018, 266, 1, 269-277.
- 13. David Dobnik, Kristina Gruden, Jana Žel, Yves Bertheau, Arne Holst-Jensen, Marko Bohanec, "Decision support for the comparative evaluation and selection of analytical methods: detection of genetically modified organisms as an example", Food analytical methods, 2018, 11, 8,2105-2122
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- 15. Vladimir Kuzmanovski, Ljupčo Todorovski, Sašo Džeroski, "Extensive evaluation of the generalized relevance network approach to inferring gene regulatory networks", GigaScience, 2018, 7, 11, giy118.

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- Senja Pollak, Geraint A. Wiggins, Martin Žnidaršič, Nada Lavrač, "Computational creativity in Slovenia", *Informatica: an international journal of computing and informatics*, 2018, 42, 1, 69-76.
- 17. Ivica Slavkov, Matej Petković, Dragi Kocev, Sašo Džeroski, "Quantitative score for assessing the quality of feature rankings", *Informatica: an international journal of computing and informatics*, 2018, **42**, 1, 43-52.
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- 21. En Fan, Weixin Xie, Jihong Pei, Keli Hu, Xiaobin Li, Vid Podpečan, "Improved Joint Probabilistic Data Association (JPDA) filter using motion feature for multiple maneuvering targets in uncertain tracking situations", *Information*, 2018, 9, 12, 322.
- 22. Valerij Grašič, Andrej Kos, Biljana Mileva Boshkoska, "Classification of incoming calls for the capital city of Slovenia smart city 112 public safety system using open Internet of Things data", *International journal* of distributed sensor networks, 2018, 14, 9, 1-12.
- 23. Dragana Miljković, Nada Lavrač, Marko Bohanec, Biljana Mileva Boshkoska, "Discovering dependencies between domains of redox potential and plant defence through triplet extraction and copulas", *International journal of intelligent engineering informatics*, 2018, 6, 1/2, 61-77.
- 24. Darja Fišer, Nikola Ljubešić, "Distributional modelling for semantic shift detection", *International journal of lexicography*, ecy011.
- 25. Marko Vidak, Ivana Jovchevska, Neja Šamec, Alja Zottel, Mirjana Liović, Damjana Rozman, Sašo Džeroski, Peter Juvan, Radovan Komel, "Metaanalysis and experimental validation identified FREM2 and SPRY1 as new glioblastoma marker candidates", *International journal of molecular sciences*, 2018, **19**, 5, 1-24.
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- 27. Biljana Mileva Boshkoska, Shaofeng Liu, Huilan Chen, "Towards a knowledge management framework for crossing knowledge boundaries in agricultural value chain", *Journal of decision systems*, 2018, **27**, suppl. 1, 88-97.
- 28. Jan Kralj, Marko Robnik Šikonja, Nada Lavrač, "HINMINE: heterogeneous information network mining with information retrieval heuristics", *Journal of intelligent information systems*, 2018, **50**, 1, 29-61.
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#### PUBLISHED CONFERENCE CONTRIBUTION

- Jan Štihec, Martin Žnidaršič, Senja Pollak, "Simplified hybrid approach for detection of semantic orientations in Economic Texts", In: Gabriella Pasi (ed.), Advances in information retrieval: 40th European Conference on IR Research, ECIR 2018, Grenoble, France, March 26-29, 2018: proceedings, (Lecture notes in computer science 10772) 2018, 692-698.
- Darja Fišer, Maria Eskevich, "The CLARIN infrastructure for open science", In: Jozef Colpaert (ed.), et al., *CALL your data: proceedings*, 2018, 125-128.
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#### MENTORING

- 1. Kristina Ban, *Multilevel complex systems approaches to computational linguistics:* doctoral dissertation, Novo Mesto, 2018 (mentor Zoran Levnajić; co-mentor Biljana Mileva Boshkoska).
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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, electronic and mobile health, and smart cities. 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 continuously collaborates with industry and contributes significantly to the inclusion of intelligent systems in products and services.

Intelligent systems simulate intelligence so that a typical user perceives them as truly intelligent. In reality, these systems use complex mechanisms and implement them on digital platforms to imitate human behaviour by exploiting raw, exponentially growing computer power. This field is somewhat broader than artificial intelligence, both are rapidly growing worldwide and enabling the development of the information society.



Prof. Matjaž Gams

Ambient intelligence is a research area aiming to introduce technology into our everyday environment in a friendly way that is undemanding for the user. Health continues to be the main domain where we apply methods of ambient intelligence. We coordinate the H2020 project HeartMan, which developed an application to help congestive-

heart-failure patients manage their condition: it monitors them with a sensing wristband, and provides advice on exercise, nutrition, etc. In 2018, the application was being evaluated in clinical trials. The objective of the H2020 project CrowdHealth is to mine health data to help craft better publichealth policies. We developed methods that can forecast time-series data and assess health risks based on such forecasts. They were used on SloFit data describing the fitness of Slovenian primary- and high-school students in cooperation with the Faculty of Sports of the University of Ljubljana. The H2020 project WellCo aims to create a virtual coach to advise older users on well being and health. We developed a web service to administer food-frequency questionnaires, and are working on nutrition monitoring with a smart watch. We are also developing methods to recognize the users' emotions from their voice, to enable an affective user interface. We started the H2020 project Insension, in which we will help people with severe intellectual disability use digital services. We are developing methods for unobtrusive, camera-based, monitoring of physiological signals, as well as methods to reason about the users' intent from observations of them and their context. We also started a Flemish-Slovenian project STRAW, whose objective is to develop stress recognition from physiological signals and to learn more about stressors in the workplace. As a doctoral research project, we developed a method that can intelligently turn sensors on and off in such a way that the energy consumption is as small as possible, but without sacrificing a lot of quality of the results obtained with these sensors. Another doctoral student is working on sensor fusion, transfer learning and multi-task learning using deep neural networks on problems of affective computing. Finally, we participated in the Sussex-Huawei Locomotion Recognition Challenge, an international competition to develop the



Figure 1: A meeting about autonomous weapons took place at the UN in Geneva in November 2018. The JSI representative analyzed the AI viewpoint.

Our teams placed first and second at the Sussex-Huawei Locomotion Recognition Challenge, an international competition to develop the best method to recognise locomotion activities from smartphone sensor data.

best method to recognise locomotion activities from smartphone sensor data, where we placed first and second. **Computational intelligence** is the 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 evolutionary computation methods. We study evolutionary algorithms for multi-objective optimization, their acceleration through parallel computing and surrogate models, visualization of their results, benchmarking methodologies, and applications in engineering design and optimization problems. In the H2020 Twinning project **SYNERGY** we are

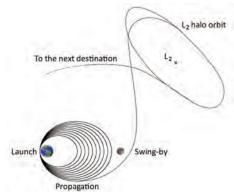


Figure 2: In the bilateral Slovenian-Japanese research project we collaborated with Shinshu University and the Japan Aerospace Exploration Agency (JAXA) on visualizing the trajectory optimization results for the Destiny space mission.

strengthening our research and innovation potential in parallelization, surrogate modelling and combining the two techniques in multi-objective optimization. The project is carried out by three partners with complementary expertise: the Jožef Stefan Institute, the University of Lille, and Cologne University of Applied Sciences. The expertise and solutions gained in this cooperation are targeted at both academic and industrial organizations, particularly those participating in the Slovenian Smart Specialisation Strategy. In 2018, the project consortium members organized the 8th International Conference on Bioinspired Optimization Methods and Their Applications, BIOMA 2018, in Paris, the Summer School on Efficient Multiobjective Optimization in Ljubljana, and the International Conference on High-Performance Optimization in Industry, HPOI 2018, in Ljubljana. We completed the bilateral Slovenian-Japanese research project aimed at enhancing the methodology of evolutionary, multi-objective optimization for real-world applications. We cooperated with Shinshu University, Nagano, and the Japan Aerospace Exploration Agency (JAXA) on visualizing the results of trajectory optimization for the Destiny space mission. Within the postdoctoral basic research project Incorporating real-world problems into the benchmarking of multiobjective optimizers we design real-world-based benchmark problems and integrate them into the state-of-the-art open-source COCO (Comparing Continuous Optimizers) platform for optimization algorithm benchmarking. The transfer of our knowledge and methods to industrial end users took place in the project Upgrade of the optimization system for steel

For a new casting device at the Štore Steel plant we developed a computer system for the multiobjective optimization of process parameters in order to improve the quality of the cast steel.



Figure 3: Organized under the Horizon 2020 project SYNERGY, the international summer school Efficient Multiobjective Optimization took place in Ljubljana during 27–31 August 2018. It was attended by 47 participants from 21 countries.



Figure 4: Results of a sorting algorithm that builds on Europeana's search engine. The left-hand side of the image shows the unprocessed results of Europeana. The right-hand side shows the sorted results after applying the image-ranking algorithm.

continuous casting (KN3) for the Štore Steel company. For a new casting device at the plant we developed a computer system for the multi-objective optimization of process parameters in order to improve the quality of the cast steel. In addition, we started an applied project A Computer System to Schedule Flexible Offers for Electricity Production and Consumption dealing with the scheduling of flexible offers for energy production and

consumption. Its goal is to develop an efficient scheduling algorithm to minimize costs due to the mismatch between available and needed energy, and assess its performance on real-world problem instances.

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 the Slovenian Smart Specialisation program EkoSMART we continue with the research activities 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 the 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 "Electronic and mobile health" (EMH), where we are the leading partner. The main goal is to develop new and innovative devices and solutions to support the elderly and chronic patients at home. One of the prototypes is a smart watch with 16 functions for elderly (ura.ijs.si). We are also involved in the Smart Specialisation program IQDOM in the field of smart buildings and homes, coordinated by Gorenje. Our focus is on the development of smart home-automation services. The aim is to apply advanced machine-learning and optimization methods to build user models and consumption profiles for housing units in order to generate control strategies that increase user comfort and, at the same time, decrease the operational costs of the smart home. Similar approaches are also applied to heat pumps. The controller learns the behaviour of the use 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 are developing an integrated tourist platform for cross-border tourist exchange, tour planning and effective communication between tourists and tourist offices. The platform will support natural language communication between the users and the system and the automatic creation of personalized itineraries based on the search concepts and preferences of the users. 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 are developing innovative applications that enable efficient search and richer visualisations of digital content related to cultural heritage from various internet sources and dedicated databases. The goal of

the **bilateral Slovenian-Macedonian research project** is to study and advance wearable and non-wearable sensors for detecting the user's physical and mental state.

In the field of **speech and language technologies** we work on speech synthesis, semantic analysis of text and question answering. Together with the companies Alpineon and Amebis we developed a new, high-quality speech synthesizer eBralec (http://ebralec.si/). The synthesizer is improved in terms of both the comprehensibility and natural perception of the speech. The software package has more than a thousand subscribers and is an indispensable tool for blind and visually-impaired users (it is the "official" speech synthesizer of the Slovenian Association for the Blind and Visually Impaired) and people with reading impairments (the Bravo association). For these users, eBralec is free of charge and can be ordered at the Library for the Blind and Visually Impaired (http://www.kss-ess.si/ebralec-sintetizator-govora-slovenskega-jezika/). eBralec is also an integral part of the DarsTraffic+ application, which provides traffic information, while its server version has been used by the National and University Library since 2017. We have also developed a service of speech synthesis for mobile devices (http://dis.ijs.si/dyslex/), which is free for anyone to use.

The **21th International Multiconference Information Society – IS 2018** (is.ijs.si) took place at the Jožef Stefan Institute from October 8 to 12, 2018. It consisted of 11 independent conferences with 200 presentations. Four conference awards were presented: for lifetime achievements ("Donald Michie and Alan Turing" award) to Prof. Saša Divjak, for current achievements in the field of information society to Assist. Prof. Marinka Žitnik, and the information strawberry (Yaskawa) and lemon (Slovenian science support) for the best and worst public information-society services.

#### Organization of conferences, congresses and meetings

- 1. Cvetković, B., Szeklicki, R., Janko, V., Lutomski, P., Luštrek, M. Real-time activity monitoring with a wristband and a smartphone. Information Fusion, 43 (2018), 77–93
- Janko, V., Luštrek, M. Using Markov chains and multi-objective optimization for energyefficient context recognition. Sensors, 18 (1) (2018), 80-1–80-17
- Medvet, E., Virgolin, M., Castelli, M., Bosman, P., Gonçalves, I., Tušar, T. Unveiling evolutionary algorithm representation with DU maps. Genetic Programming and Evolvable Machines, 19 (3) (2018), 351–389
- 4. Tavčar, A., Gams, M. Surrogate-agent modeling for improved training. Engineering Applications of Artificial Intelligence, 74 (2018), 280–293

#### Awards and appointments

- 1. Jani Bizjak, Matjaž Gams, Anton Gradišek: Best innovation from public research organizations, TEE-The ultimate European assistant for the elderly, at IS 2018
- 2. Jani Bizjak, Vid Drobnič, Matjaž Gams, Martin Gjoreski, Vito Janko, Mitja Luštrek, Matej Marinko, Miha Mlakar, Nina Reščič, Gašper Slapničar: SHL Challange – Sussex-Huawei Locomotion and Transportation Recognition Challenge, 1st Place Award; Singapore; Dr. Hristijan Gjoreski, University of Sussex (UK) & Ss. Cyril and Methodius University (MK), Dr. Lin Wang, University of Sussex (UK), Dr. Daniel Roggen, University of Sussex (UK), Dr. Kazuya Murao, Ritsumeikan University (JP), Dr. Tsuyoshi Okita, Kyushu Institute of Technology (JP); method for recognition of locomotion activity from smartphone sensors
- 3. Vid Drobnič, Matjaž Gams, Martin Gjoreski, Vito Janko, Mitja Luštrek, Matej Marinko, Nina Reščič, Gašper Slapničar: SHL Challange Sussex-Huawei Locomotion and Transportation Recognition Challenge, 2nd Place Award; Singapur; Dr. Hristijan Gjoreski, University of Sussex (UK) & Ss. Cyril and Methodius University (MK), Dr. Lin Wang, University of Sussex (UK), Dr. Daniel Roggen, University of Sussex (UK), Dr. Kazuya Murao, Ritsumeikan University (JP), Dr. Tsuyoshi Okita, Kyushu Institute of Technology (JP); method for recognition of locomotion activity from smartphone sensors

#### Organization of conferences, congresses and meetings

- 1. 32nd Slovenian Workshop on Nature-Inspired Algorithms, AVN, Donačka gora, 25. 5. 2018
- 2. Session Evolutionary Computation in Practice (ECiP) at the Genetic and Evolutionary Computation Conference, GECCO 2018, Kyoto, Japan, 17. 7. 2018
- 3. Genetic and Evolutionary Computation Conference, GECCO 2018, Kyoto, Japan, 15.-19. 7. 2018



Figure 5: At the Sussex-Huawei world-open competition presented at the Ubicomp conference in Singapore, where data from mobile phones were used to determine the type of transportation, two teams achieved the first and the second place. The estimated probability of such an event was 0.004, and therefore it is highly significant.

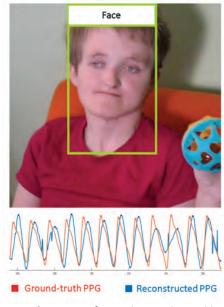


Figure 6: Prototype of an application that enables monitoring of physiological parameters, such as heart rate, using a camera. Heart rate is evaluated using the reconstructed PPG signal, which describes periodic changes of skin color in line with the beating of the heart.



- 4. BBOB (Blackbox Optimization Benchmarking) workshop at the Genetic and Evolutionary Computation Conference, GECCO 2018, Kyoto, Japan, 15. 7. 2018
- 5. GBEA (Game-Benchmark for Evolutionary Algorithms) workshop at the Genetic and Evolutionary Computation Conference, GECCO 2018, Kyoto, Japan, 15. 7. 2018
- GECCO Job Market at the Genetic and Evolutionary Computation Conference, GECCO 2018, Kyoto, Japan, 17. 7. 2018
- 7. 21th International Multiconference Information Society, IS 2018, Ljubljana, Slovenia, 8. –14. 10. 2018; independent conferences:
  - International conference on cognitonics
  - Cognitive science
  - Collaboration, software and services in information society
  - Data mining and data warehouses
  - Facing demographic challenges
  - International conference of transfer of technologies
  - High-Performance Optimization in Industry, HPOI 2018
  - Slovenian conference on artificial intelligence
  - Workshop AS-IT-IC
  - Workshop electronic and mobile health and smart cities
- 8. 33rd Slovenian Workshop on Nature-Inspired Algorithms, AVN, Ljubljana, 14. 12. 2018

## INTERNATIONAL PROJECTS

- COST TD1405; ENJECT, European Network for the Joint Evaluation of Connected Health Technologies Dr. Božidara Cvetković
  - Cost Office
- 2. CardioRNA Catalysing Transcriptomics Research in Cardiovascular Disease Dr. Mitja Luštrek
- Cost Association Aisbl 3. H2020 - IN LIFE; INdependent Living support Functions for the Elderly
- Prof. Matjaž Gams European Commission
- 4. H2020 eHERITAGE; Expanding the Research and Innovation Capacity in Cultural Heritage Virtual Reality Applications
- Prof. Matjaž Gams European Commission
- H2020 CrowdHEALTH; Collective Wisdom Driving Public Health Policies Dr. Mitja Luštrek
- European Commission
- 6. H2020 INSENSION; Personalized Intelligent Platform Enabling Interaction with Digital Services to Individuals with Profound and Multiple Learning Disabilities Dr. Mitja Luštrek
- European Commission 7. H2020 - WellCo; Wellbeing and Health Virtual Coach Dr. Mitja Luštrek
- European Commission
- H2020 HeartMan; Personal Decison Support System for Heart Failure Management Dr. Mitja Luštrek European Commission
- H2020 SYNERGY, Synergy for Smart Multi-Objective Optimisation Prof. Bogdan Filipič
- European Commission
- Advanced Methodology of Evolutionary Multi- and Many-Objective Optimization for Real-World Applications Prof. Bogdan Filipič
- Slovenian Research Agency
- 11. Patient Health Prediction and Diagnostics based on Sensor Data and Machine Learning Prof. Matjaž Gams
  - Slovenian Research Agency

## **RESEARCH PROGRAM**

1. Artificial Intelligence and Intelligent Systems Prof. Matjaž Gams

## R & D GRANTS AND CONTRACTS

- Disentangling the sources and context of daily work stress: a comprehensive real-time modelling study using wearbles and technological detections Dr. Mitia Luštrek
- Intelligent home of the new generation designed on smart appliances and wood Prof. Matjaž Gams
- Ministry of Education, Science and Sport 3. Smart City Ecosystem – EkoSmart
- Prof. Matjaž Gams
- Ministry of Education, Science and Sport
- 4. Food for future F4F
- Dr. Mitja Luštrek Ministry of Education, Science and Sport
- Austrian-Slovenian Intelligent Tourist Information Center (AS-IT-IC)
   Prof. Matjaž Gams
- Government Office for Development and European Cohesion Policy
- 6. Strategic Research & Innovation Partnership (SRIP) Smart Cities and Communities Prof. Matjaž Gams
- Ministry of Economic Development and Technology
- 7. Self-management of physical and mental fitness of older workers Dr. Mitja Luštrek
- Ministry of Education, Science and Sport
- 21st International Multiconference Information Society 2018, IS 2018, Ljubljana, Slovenia, 8 October 2018 - 12 October 2018 Prof. Matjaž Gams

## NEW CONTRACTS

- A Computer System to Schedule Flexible Offers for Electricity Production and Consumption Prof. Bogdan Filipič
- Inea d. o. o.
- Implementing services within the CityVOICE project Dr. Tomaž Šef
- Amebis, d. o. o., Kamnik

## VISITORS FROM ABROAD

- Dr. Mihai Duguleana, Department of Automotive and Transport Engineering, Transilvania University of Brasov, Brasov, Romania, 29.–31. 1. 2018
- Dr. Marcello Carrozzino, PERCRO Perceptual Robotics Laboratory, Scuola Superiore S. Anna, Pisa, Italy, 29.–31. 1. 2018
- 3. Prof. Dr. Hernán Aguirre, Taishi Ito, Shinshu University, Nagano, Japan, 14.–16. 3. 2018 A Prof. Dr. Akira Ovama, Hiradki Fukumata, Japan Agrospace, Evalentijan Agnory (JAXA)
- Prof. Dr. Akira Oyama, Hiroaki Fukumoto, Japan Aerospace Exploration Agency (JAXA), Sagamihara, Japan, 8.–10. 4. 2018

- 5. Peter Guillaume, Richard Louvancour, Yanis Kettou, Polvtech Paris UPMC, Paris, France, 14. 5. - 28. 7. 2018
- Gaspard Delaurelle, Polytech Paris UPMC, Paris, France 21. 5.-27. 7. 2018 6.
- Prof. Dr. Luca Bortolussi, Dr. Eric Medvet, University of Trieste, Trieste, Italy, 13. 6. 2018 7
- Nicolas Cheron, Polytech Paris Sorbonne, Paris, France, 18. 6.-18. 8. 2018. 9
- Marija Trajanoska, Faculty of Electrical Engineering and Information Technologies, Skopje, Republic of Macedonia, 23. 7.-16. 9. 2018
- 10. Dr. Octavian Machidon, Department of Electronics and Computers, Transilvania University of Brasov, Brasov, Romania, 13.-31. 8. 2018
- 11. Prof. Dr. Enrique Alba, University of Malaga, Malaga, Spain, 28. 8. 2018
- 12. Dr. Pavel Krömer, Technical University of Ostrava, Ostrava, Czechia, 28. 8. 2018

### STAFF

#### Researchers

- Dr. Erik Dovgan 1.
- Prof. Bogdan Filipič 2
- Prof. Matjaž Gams, Head 3.
- 4 Dr. Anton Gradišek
- 5. Dr. Mitia Luštrek
- 6. Dr. Miha Mlakar
- Dr. Tomaž Šef
- 8 Dr. Tea Tušar
- Postdoctoral associates
- Dr. Matej Guid
- 10. Dr. Rok Piltaver\*
- 11. Dr. Aleksander Pivk\*
- 12. Dr. Aleš Tavčar
- Postgraduates
- 13. Dr. Božidara Cvetković, 09.07.18, transferred to Department E8
- 14. Martin Gjoreski, B. Sc.
- 15. Vito Janko, B. Sc.
- 16. Tine Kolenik, B. Sc.
- 17. Tomaž Kompara\*, B. Sc.
- 18. Dr. Jana Krivec\*
- 19. Damjan Kužnar, B. Sc., left 02.01.18
- 20. Aljoša Vodopija, B. Sc.
- 21. Jernej Zupančič, B. Sc.

- 13. Hiroaki Fukumoto, Japan Aerospace Exploration Agency (JAXA), Sagamihara, Japan. 5.-8.10.2018
- 14. Prof. Dr. Thomas Bartz-Beielstein, Beate Breiderhoff, Frederik Rehbach, Jörg Stork, Cologne University of Applied Sciences (TH Köln), Gummersbach, Germany, 8. 10. 2018
- 15. Dr. Wellington Rodrigo Monteiro, Pontifical Catholic University of Paraná, Curitiba, Brazil, 8, 10, 2018
- 16. Prof. Dr. El-Ghazali Talbi, University of Lille, Lille, France, 8. 10. 2018
- Prof. Dr. Boris Naujoks, Cologne University of Applied Sciences (TH Köln), 17.
- Gummersbach, Germany, 11.-14. 12. 2018 18. Vanessa Volz, Queen Mary University of London, London, Great Britain, 11.-14. 12. 2018

#### Technical officers

- 22. Andrejaana Andova, B. Sc.
- 23. Luka Colarič, B. Sc., left 01.03.18
- 24. Mateja Drnovšek, B. Sc.
- 25. Gregor Grasselli, B. Sc. 26. Gašper Slapničar, B. Sc.
- 27. Maj Smerkol, B. Sc., left 01.10.18
- 28. Jure Šorn\*, B. Sc., left 01.05.18
- 29. Jakob Valič, B. Sc.
- Technical and administrative staff
- 30. Jani Bizjak, B. Sc.
- 31. Matej Cigale, B. Sc.
- 32. Grigory Evseev, B. Sc., left 16.05.18
- 33. Vesna Koricki, B. Sc.
- 34. Mitja Lasič
- 35. Liljana Lasič
- 36. Junoš Lukan, B. Sc.
- 37. Blaž Mahnič, B. Sc.
- 38. Pavel Maslov, B. Sc., left 17.10.18
- 39. Nina Reščič, B. Sc. 40. Luka Stepančič, B. Sc., left 01.02.18
- 41. Lana Zemljak

Note:

\* part-time ISI member

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- 5. Erik Dovgan, Cristina Knapic, Massimo Sponza, Riccardo Smareglia, "A new archival infrastructure for highly-structured astronomical data", Experimental astronomy, 2018, 45, 1, 41-55.
- Eric Medvet, Marco Virgolin, Mauro Castelli, Peter Bosman, Ivo Gonçalves, Tea Tušar, "Unveiling evolutionary algorithm Tušar, algorithm representation with DU maps", Genetic programming and evolvable machines, 2018, 19, 3, 351-389.
- 7. Gašper Slapničar, Mitja Luštrek, Matej Marinko, "Continuous blood pressure estimation from PPG signal", Informatica: an international journal of computing and informatics, 2018, 42, 1, 33-42.

- 8. Martin Gjoreski, Mitja Luštrek, Matjaž Gams, Blagoj Mitrevski, "An interdomain study for arousal recognition from physiological signals", Informatica: an international journal of computing and informatics, 2018. 42, 1, 61-68.
- 9. Alen Ajanović, Andrej Ulčar, Ana Marija Peterlin, Karolina Počivavšek, Gašper Fele-Žorž, Anton Gradišek, Matjaž Gams, Mojca Matičič, "Application for viral hepatitis infection risk assessment - HEPY", Informatica: an international journal of computing and informatics, 2018, 42, 2, 279-281.
- 10. Božidara Cvetković, Robert Szeklicki, Vito Janko, Przemyslaw Lutomski, Mitja Luštrek, "Real-time activity monitoring with a wristband and a smartphone", Information fusion, 2018, 43, 77-93.
- Tine Kolenik, "Seeking after the glitter of intelligence in the base metal 11 of computing: the scope and limits of computational models in researching cognitive phenomena", Interdisciplinary description of complex systems, 2018, 16, 4, 545-557.
- 12. Rok Piltaver, Hristijan Gjoreski, Matjaž Gams, "Identifying a person with door-mounted accelerometer", Journal of ambient intelligence and smart environments, 2018, **10**, 5, 361-375.
- 13. Uroš Zavrtanik, Junoš Lukan, Remy Loris, Jurij Lah, San Hadži, "Structural basis of epitope recognition by heavy-chain camelid antibodies", Journal of molecular biology, 2018, 430, 21, 4369-4386.
- 14. Anton Gradišek, Mitja Krnel, Mark Paskevicius, Bjarne R. S. Hansen, Torben Rene Jensen, Janez Dolinšek, "Reorientational motions and ionic conductivity in  $(\mathrm{NH}_4)_2\mathrm{B}_{10}\mathrm{H}_{10}$  and  $(\mathrm{NH}_4)_2\mathrm{B}_{12}\mathrm{H}_{12}$  , The journal of physical chemistry. C, Nanomaterials and interfaces, 2018, 122, 30, 17073-17079.
- 15. Jana Krivec, Primož Rakovec, "Cognitive behavioral profile of stress experience among Slovenian students", Kairos: slovenska revija za psihoterapijo, 2018, 12, 1/2, 67-86.

- 16. Clarissa P. C. Gomes, Antonio Salgado-Somoza, Ester E. Creemers Creemers, Yvan Devaux Dieterich, Mitja Luštrek, On behalf of the CardiolincTM network, "Circular RNAs in the cardiovascular system", *Non-coding RNA research*, 2018, **3**, 1, 1-11.
- 17. Miha Mlakar, Paolo Emilio Puddu, Maja Somrak, Silvio Bonfiglio, Mitja Luštrek, On behalf of the the Chiron and HeartMan research projects, "Mining telemonitored physiological data and patient-reported outcomes of congestive heart failure patients", *PloS one*, 2018, **13**, 3, e0190323.
- Vito Janko, Mitja Luštrek, "Using markov chains and multi-objective optimization for energy-efficient context recognition", *Sensors*, 2018, 18, 1, 80.
- Monika Simjanoska, Martin Gjoreski, Matjaž Gams, Ana Madevska Bogdanova, "Non-invasive blood pressure estimation from ECG using machine learning techniques", *Sensors*, 2018, 18, 4, 1160.
- Robert Oravecz, Jerica Penko, Jana Suklan, Jana Krivec, "Prevalence of post-traumatic stress disorder, symptomatology and coping strategies among Slovene medical emergency professionals", *Sigurnost*, 2018, 60, 2, 117-127.

#### PUBLISHED CONFERENCE CONTRIBUTION

- Vito Janko, Mitja Luštrek, "Choosing duty-cycle parameters for context recognition", In: Jason J. Jung (ed.), *The 14th International Conference on Intelligent Environments, IE'18, 25th-28th June 2018, Rome, Italy*, 2018.
- Junoš Lukan, Martin Gjoreski, Heidi Mauersberger, Annekatrin Hoppe, Ursula Hess, Mitja Luštrek, "Analysing physiology of interpersonal conflicts using a wrist device", In: Achilles Kameas (ed.), Kostas Stathis (ed.), Ambient Intelligence: 14th European Conference, Aml 2018, Larnaca, Cyprus, November 12-14, 2018: proceedings, (Lecture notes in computer science 11249) 2018, 162-167.
- 3. Jani Bizjak, Matjaž Gams, "Adaptive filtering combined with deep ensembles for better arrhythmia detection", In: *BOOM 2018*, 3rd International Workshop on Biomedical Informatics with Optimization and Machine Learning in conjunction with 27th International joint Conference on Artificial Intelligence (IJCAI), July 2018, Stockholm, Sweden as part of the Federated AI Meeting (FAIM) 2018.
- 4. Anton Gradišek, Miha Mlakar, Matej Cigale, Luka Lajovic, Mitja Luštrek, Maroje Sorić, Gregor Starc, Bojan Leskošek, Gregor Jurak, "Physical fitness forecasting and risk estimation in slovenian schoolchildren", In: Arie Hasman (ed.), Data, informatics and technology: an inspiration for improved healthcare, ICIMTH 2018, [International Conference on Informatics, Management and Technology in Healthcare, 6-8 July 2018 in Athens, Greece], (Studies in health technology and informatics 251) 2018, 125-128.
- Jernej Zupančič, Oliver A. Tazi, Blaž Mahnič, Gregor Grasselli, "AS-IT-IC databases", In: Matjaž Gams (ed.), Jernej Zupančič (ed.), AS-IT-IC Workshop: proceedings of the 21st International Multiconference Information Society - IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume E, 2018, 14-17.
- 6. Jernej Zupančič, Matjaž Gams, "Austrian-Slovenian Intelligent Tourist Information: project progress report 2018", In: Matjaž Gams (ed.), Jernej Zupančič (ed.), AS-IT-IC Workshop: proceedings of the 21st International Multiconference Information Society - IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume E, 2018, 5-9.
- 7. Gregor Grasselli, "e-Tourist 2.0: an adaptation of the e-Tourist for the AS-IT-IC project", In: Matjaž Gams (ed.), Jernej Zupančič (ed.), AS-IT-IC Workshop: proceedings of the 21st International Multiconference Information Society IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume E, 2018, 20-22.
- Gregor Grasselli, Jernej Zupančič, "Tourism related ICT tools: project progress report 2018", In: Matjaž Gams (ed.), Jernej Zupančič (ed.), AS-IT-IC Workshop: proceedings of the 21st International Multiconference Information Society - IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume E, 2018, 10-13.
- 9. Mateja Drnovšek, Matjaž Gams, "EMZ in EkoSMART-asistent", In: Matjaž Gams (ed.), Aleš Tavčar (ed.), Workshop Electronic and mobile health and smart cities: proceedings of the 21st International Multiconference Information Society IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume I, 2018, 11-14.
- 10. Matej Cigale, Anton Gradišek, Miha Mlakar, Mitja Luštrek, "Forecasting the physical fitness and all-cause mortality based of schoolchildren's fitness measurements", In: Matjaž Gams (ed.), Aleš Tavčar (ed.), Workshop Electronic and mobile health and smart cities: proceedings of the 21st International Multiconference Information Society - IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume I, 2018, 69-72.

- 11. Aleš Tavčar, Matjaž Gams, "Napredni pogovorni svetovalci", In: Matjaž Gams (ed.), Aleš Tavčar (ed.), Workshop Electronic and mobile health and smart cities: proceedings of the 21st International Multiconference Information Society IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume I, 2018, 53-56.
- 12. Tomaž Šef, "Postopki in priporočila za izgradnjo govorne zbirke za potrebe sinteze slovenskega govora", In: Matjaž Gams (ed.), Aleš Tavčar (ed.), Workshop Electronic and mobile health and smart cities: proceedings of the 21st International Multiconference Information Society IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume I, 2018, 46-49.
- 13. Mateja Drnovšek, Matjaž Gams, Aleš Tavčar, Gregor Grasselli, "Pregled asistentov IJS E9", In: Matjaž Gams (ed.), Aleš Tavčar (ed.), Workshop Electronic and mobile health and smart cities: proceedings of the 21st International Multiconference Information Society - IS 2018, 8-12 October, 2018, [Ljubljana, Slovenia]: volume I, 2018, 15-19.
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- 20. Aljoša Vodopija, Tea Tušar, Bogdan Filipič, "Comparing black-box differential evolution and classic differential evolution", In: *GECCO 2018, the Genetic and Evolutionary Computation Conference Companion a recombination of the 27th International Conference on Genetic Algorithms (ICGA) and the 23rd Annual Genetic Programming Conference (GP), July 15th 19th 2018, Kyoto, Japan, 2018, 1537-1544.*
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- 44. Martin Gjoreski, Mitja Luštrek, Matjaž Gams, "Multi-task ensemble learning for affect recognition", In: UbiComp/ISWC'18 adjunct, 2018, 553-558.
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- 47. Martin Gjoreski, Vito Janko, Nina Reščič, Miha Mlakar, Mitja Luštrek, Jani Bizjak, Gašper Slapničar, Matej Marinko, Vid Drobnič, Matjaž Gams, "Applying multiple knowledge to Sussex-Huawei locomotion challenge", In: UbiComp/ISWC'18 adjunct, 2018, 1488-1496.
- 48. Vito Janko, Nina Reščič, Miha Mlakar, Vid Drobnič, Matjaž Gams, Gašper Slapničar, Martin Gjoreski, Jani Bizjak, Matej Marinko, Mitja Luštrek, "A new frontier for activity recognition: the Sussex-Huawei locomotion challenge", In: UbiComp/ISWC'18 adjunct, 2018, 1511-1520.
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#### MENTORING

1. Božidara Cvetković, *Multi-model semi-supervised learning for personalisation:* doctoral dissertation, Ljubljana, 2018 (mentor Mitja Luštrek; 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 programmes. Our research results are incorporated into projects for industry and for the regulatory authority, as well as in under-graduate 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 project SESAME that is dedicated to the thermal hydraulics of liquid metals. Simulations are being performed in a geometry of a backward-facing step, with a heater attached below the floor after the step. Results obtained at low Reynolds numbers are available to other project partners for the validation of turbulent heat-transfer models.

As part of the analysis of jet impingement cooling, the uncertainty of Large Eddy Simulation (LES) results Prof. Leon Cizelj was assessed. Adequate accuracy for the benchmarking of less-accurate simulation methods was demonstrated; therefore, the assessment study of computationally less-demanding statistical turbulence models was conducted. A significant improvement in the prediction of flow unsteadiness with the Scale-Adaptive Simulation approach was observed compared to standard Unsteady Reynolds Averaged Navier-Stokes (URANS) models.

Conjugate heat-transfer simulations were performed with a wallresolved LES model, using the open-source code Code\_Saturne, in collaboration with Electricité de France (EDF). The capabilities of LES models for detailed simulations of the turbulent heat transfer in geometries, where penetration of turbulent fluctuations into solid walls must be predicted, were validated. The work was concluded with the development of a new

tested.

correlation for temperature turbulence dissipation jump at the fluid-solid interface. The correlation is based on LES results and is useful for RANS turbulent models that are being used in conjugate heat-transfer simulations.

In the field of the research of separated upward air-water flow in a vertical pipe, the influence of interface compression in simulations using the two-phase flow homogeneous mixture model within the open-source Computational Fluid Dynamics (CFD) code OpenFOAM was analysed.

Basic phenomena of vapour explosion, which might occur during a hypothetical severe accident in a nuclear power plant (NPP), if the hot reactor-core melt comes into contact with the coolant, were investigated. The study of

vapour explosions in stratified melt-water configurations was continued. The PULiMS and SES experiments (Royal Institute of Technology, Sweden) were analysed using the MC3D code (Institut de Radioprotection et de Sûreté Nucléaire - IRSN, France). Three-dimensional analyses showed that a longer explosion duration for experiments with strong explosions cannot be fully predicted by the present simulation models of the premixed layer. A mechanistic model of the premixing layer was proposed, based on theoretical research and recent experiments.

The potential of vapour explosions during the melt-sodium interaction was also further investigated. We have started with a numerical investigation of the heat transfer around the melt fragments in sodium using the NEPTUNE\_CFD code (EDF). We performed a numerical analysis of single-phase heat transfer around melt fragments in sodium or water and compared the results with correlations for the single-phase flow of water and sodium. Furthermore, the effect of sodium sub-cooling on the initial conditions for potential energetic fuel-sodium interaction in characteristic experimental geometry was analysed using the MC3D code. The results indicate that the potential of a vapour explosion in sodium is lower than in water.

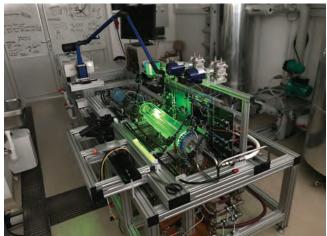


Figure 1: Experimental facility for research on fluid mechanics and heat transfer.



The newly built experimental facility for fluid mechanics and heat transfer was successfully

In the field of hydrogen distribution in NPP containment, an experiment on the erosion of a helium layer in the upper part of a cylindrical vessel, jointly proposed by the JSI, Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA, France), IRSN and EDF, was performed at the Nuclear Power Institute of China on the MCTHBF facility (Mid-size Containment Thermal-Hydraulic Behavior Facility). The experiment was later simulated with the OpenFOAM code. Also, conditions of experiments, performed on the PANDA facility (Paul Scherrer Institute - PSI, Switzerland) were scaled-up to the Krško NPP containment.

In the field of hydrogen combustion, simulations of experiments, performed on the THAI facility (Becker Technologies, Germany) and of the UFPE experiment, proposed by the JSI and performed on the HYKA A2 facility (Karlsruhe Institute of Technology, Germany) with the CFD Fluent code and the ETFC (Extended Turbulent Flame speed Closure) model, were continued. Hydrogen combustion in the extended THAI+ facility was also simulated with the system code ASTEC (IRSN) within the ASCOM project. The ability of the ASTEC code, developed for the simulation of severe accidents in real conditions, for the simulation of flame propagation through containment compartments, may thus be evaluated.

Research on pool scrubbing, which can be used for gas decontamination during a severe accident, was initiated within the IPRESCA project. The gas flows through a liquid pool as bubbles, while fission products in the form of particles (aerosols and larger) move from the bubbles into the liquid. The scrubbing process under the experimental conditions of POSEIDON II (PSI) was simulated with a multi-fluid model (air, water, particles in bubbles, particles in water) using the OpenFOAM code.

The construction of the experimental laboratory for fluid mechanics and heat-transfer research was continued. This year's focus was on the installation of instruments and on the integration of the test section in the loop. The test facility, which will allow instantaneous measurements of the velocity field where local heat-transfer coefficients during diabatic two-phase flow are measured, was successfully tested for the first time. This marks the beginning of experimental activities in the division. However, before performing valuable experiments, thermal balances must be closed and the calibration must be carried out.

#### Thermal-hydraulic safety analyses

The LOFT facility is a 50 MW<sub>th</sub> two-loop pressurized-water reactor, which was designed to study the thermalhydraulic response during a variety of accident scenarios. The LOFT experiment L9–1/L3–3, which represents a loss of feedwater with multiple failures and a sequentially induced small break loss-of-coolant accident, was simulated with the latest RELAP5/MOD3.3 system computer code. The code was assessed for four phases: initial heatup phase, spray and power operated relief valve cycling phase, blowdown phase and recovery phase.

The thermal response of a multi-purpose probe for plasma diagnostics in small fusion tokamaks was investigated. A postulated helium ingress event in the DEMO fusion reactor foresees a failure of the magnets cryogenic cooling line, leading to helium leakage into the cryostat. During and after this ingress, heat is transferred from the warm cryostat to the cold magnet structures. Due to the large temperature difference between the helium and the cryostat, the natural convection

of helium is established, which causes a significant local cool-down of the cryostat walls. A simulation of natural convection in the cryostat following helium ingress was performed to determine the heat transfer and temperature distribution in the cryostat walls. These analyses were related to the European nuclear fusion project WPPMI.

The thermal response of a multi-purpose probe for plasma diagnostics in small fusion tokamaks was studied in the frame of the European fusion project WP-MST2. The transient response of the probe head during three consecutive immersions into the hot plasma was simulated. The results showed that critical temperatures in the vital parts of the probe head are not exceeded in any of the operational scenarios.

#### Structural safety analyses

A new top-down approach was used to study the influence of plastic slip localisation, as observed experimentally in deformed low stacking-fault-energy (or neutron-irradiated) austenitic stainless steels, on local intergranular stress amplitudes. In this respect, a new tool was developed to generate polycrystalline aggregate models with

#### A simple phenomenological law was identified that allows an easy estimation of intergranular normal stress concentrations in a general untextured metallic polycrystal.

additional narrow lamella-like regions embedded within the grains that can be activated during a simulation and accumulate considerably more plastic strain than the neighbouring bulk.

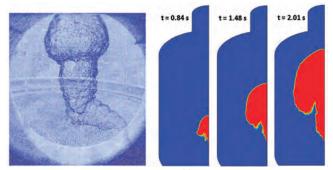
In cooperation with CEA, studies continued in the field of grain-boundary stress investigation for various polycrystalline materials under different macroscopic loading conditions. A new empirical relation was identified

to estimate the scatter of intergranular stresses present in a general untextured (random) polycrystal. Using this scatter, the probability for crack initiation may now be quickly and reliably obtained in the considered polycrystals. Also, in cooperation with CEA, a new study was initiated in order to verify the assumption that locations in

a material with the largest intergranular normal stresses strongly correlate with the locations of intergranular

micro-crack initiation. An in-house tool was developed to automatically build realistic finite-element meshes from the measured electron backscatter diffraction maps of proton-irradiated stainless-steel specimens to be provided by CEA.

Within the European project SOTERIA and in collaboration with IRSN and the Centre National de la Recherche Scientifique (CNRS, France), a comparison between Finite Element Method simulations and Fast Fourier Transform based simulations was performed on monocrystalline and polycrystalline simulations of irradiated austenitic stainless steel. Tensile and average grain-boundary stress responses of single-crystal, bi-crystal and polycrystal models, all with periodic boundary conditions, were simulated and compared between the two methods.



*Figure 2: Photograph and simulation of flame propagation during UFPE experiment on hydrogen combustion.* 

We also participated in the European fusion project WPDC (diagnostic

and control) where a finite-element analysis on electromagnetic disruption forces was carried out for the divertor thermo-current measurement diagnostics in the DEMO fusion reactor. A maximum allowed pipe current was estimated, assuming realistic material properties and magnetic fields inside the tokamak, and also true geometries of the divertor cassette and water-cooling pipes fixed to the cassette.

#### Probabilistic safety assessment

Operational events of failure or deficiency of an essential power supply system were identified and analyzed in four databases of operational events. The main findings from the evaluation of the events were presented, as well as observations of the causes resulting in the events and potential actions that can decrease their number and consequences.

A probabilistic risk-assessment method for the security of supply in gas networks supported by physical models was developed. The method is based on a procedure for the automatic generation of fault trees, which estimates the probability of disruption of the gas delivery from terminals/ storages to each consumer node in the network. The method, which allows

Identification and analysis of operational events of failure or deficiency of an essential powersupply system was performed.

probabilistic analyses of the availability of the demand nodes and of the overall availability of the gas network, was tested on the reduced United Kingdom network.

The European NARSIS project aims to extend present probabilistic safety-assessment methodologies to extreme events with very low frequencies. Contributions to the project related to the better characterization of natural external hazards and their combinations were prepared.

#### Technical cooperation, consulting services and education

In 2018, the Reactor Engineering Division cooperated in projects for industry and the state administration as well. As an authorized institution for radiation and nuclear safety, we prepared two independent evaluations on the implementation of the emergency control room in the Krško NPP. The instalation of new instruments, systems and components leads to changes in the Krško NPP Updated Safety Analysis Report. We also prepeared an independent opinion on outage and refueling activities in the Krško NPP.

For the Slovenian nuclear safety administration, we analysed the influence of the Krško NPP safety upgrade programme on the severe accident management guidelines. For the utility company GEN energija, we described and compared the safety characteristics of seven candidate reactors for the potential second unit of the Krško NPP.

Researchers of the department represent the core staff of the Chair for nuclear engineering at the Faculty of Mathematics and Physics at the University of Ljubljana, and are involved in nuclear engineering undergraduate, master and doctoral studies. The programmes are associated with the European Nuclear Education Network (ENEN).

#### Some outstanding publications in the past year

- 1. E. Flageul, I. Tiselj, Convergence rate of individual and global quantities in direct numerical simulations, Physics of Fluids 30 (2018), 111704-1-111704-4
- J. Kokalj, M. Uršič, M. Leskovar, L. Piar, R. Meignen, Modelling of debris bed reflooding in PEARL experimental facility with MC3D code, Nuclear Engineering and Design 330 (2018), 450-462
- O. Costa Garrido, B. Končar, R. Brown, C. Bachmann, Pre-conceptual design of DEMO upper port duct bellows, Fusion Engineering and Design 136B (2018), 1130-1134
- 4. S. El Shawish, J. Hure, Intergranular normal stress distributions in untextured polycristalline aggregates, European Journal of Mechanics A 72 (2018), 354-373



5. A. Volkanovski, M. Peinador Veira, Analysis of loss of essential power system reported in nuclear power plants, Science and Technology of Nuclear Installations 2018 (2018), 3671640-1-3671640-21

#### Awards and appointments

- 1. Tadej Holler, Romain Grosseuvres, Alexandre Bleyer, Ludovic Maas, Mantas Povilaitis: "ETSON Award 2018" for collaborative paper of junior experts (ETSON Award, Brussels, Belgium), European Technical Safety Organisations Network, for the paper "Temperature conditions effect on hydrogen-air flame propagation in the ENACCEF2 experimental facility"
- Tadej Holler, Ed M.J. Komen, Ivo Kljenak: Young author award (NENE 2018 conference, Portorož, Slovenia), Nuclear Society of Slovenia, for the paper "Weighted laminar flame speed approach to simulating large-scale hydrogen deflagration experiment"
- Janez Kokalj, Matjaž Leskovar, Mitja Uršič: Best poster award (NENE2018 conference, Portorož, Slovenia), Nuclear Society of Slovenia, for the paper "Model for premixed layer formation in stratified melt-coolant configuration"

#### Organization of conferences, congresses and meetings

- 1. SESAME/Myrte Cluster Progress Meeting, Jožef Stefan Institute Reactor Center, 20.-22. March 2018
- 2. European Atomic Energy Society (EAES) meeting, Evropa Hotel, Celje, Slovenia, 2.-6. June 2018
- Training course "Requirements and safety evaluation of research reactors", Jožef Stefan Institute Reactor Center, 1.-5. October 2018
- Seminar on Piping Issues in ATLAS+ (SEPIA), Slovene Ethnographic museum, Ljubljana, Slovenia, 23.-24. October 2018
- 5. Opening of the laboratory for two-phase flow studies, Jožef Stefan Institute Reactor Center, 3. December 2018

### INTERNATIONAL PROJECTS

- 1. Analysis to support Implementation in Practise of Articles 8a-8c of Directive 2014/87/ Euratom
- Prof. Leon Cizelj

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 Prof. Leon Cizelj
- Iter-consult Srl Independent
- H2020 SESAME; thermal hydraulics Simulations and Experiments for the Safety Assessment of MEtal cooled reactors Prof. Iztok Tiseli
- European Commission
- H2020 SOTERIA; Safe Long Term Operation of Light Water Reactors based on Improved Understanding of Radiation Effects in Nuclear Structural Materials Prof. Leon Cizelj European Commission
- H2020 ANNETTE; Advanced Networking for Nuclear Education and Training and Transfer of Expertise
  - Prof. Leon Cizelj
  - European Commission
- H2020 ATLASplus; Advanced Structural Integrity Assessment Tools for Safe Long Term Operation
  - Prof. Leon Cizelj
- European Commission
- H2020 NARSIS; New Approach to Reactor Safety Improvements Dr. Andrija Volkanovski European Commission
- H2020 ENENplus; Attract, Retain and Develop New Nuclear Talents Beyond Academic Curricula
- Asst. Prof. Ivo Kljenak European Commission
- 9. H2020 EUROfusion Research Unit Administration and Services RU FU
- Dr. Boštjan Končar European Commission
- H2020 EUROfusion Education-ED-FU Dr. Boštjan Končar
- European Commission 11. H2020 EUROfusion - Plant Level System Engineering-PMI-PPPT-FU
- Dr. Boštjan Končar European Commission
- 12. H2020 EUROfusion JET Enhancements-JET4-FU, EUROFUSION

Dr. Boštjan Končar European Commission

- H2020 EUROfusion Diagnostic and Control-WPDC-PPPT-FU Dr. Samir El Shawish European Commission
- 14. Experimental and Numerical Studies of High Temperature Gas-Cooled Reactors Prof. Leon Cizelj
- Slovenian Research Agency 15. SNETP General Assembly - Member of the Governing Board Prof. Leon Cizelj
  - Slovenian Research Agency General Assembly of the ENEN Association - President of the Governing Board
  - Prof. Leon Cizelj Slovenian Research Agency

### RESEARCH PROGRAM

1. Reactor engineering Prof. Leon Cizelj

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

- 1. Pressurization process during vapour explosion in sodium cooled fast reactors Dr. Mitja Uršič
- Efficient cooling concepts for high heat flux components in fusion reactor Dr. Boštjan Končar
- Investigation of turbulent heat transfer in an annulus through advanced experimental and computational methods Prof. Iztok Tiseli
- 4. Financing of project visits at the Slovenian higher education institutions pilot project - dr. Volkanovski
- Dr. Andrija Volkanovski Javni štipendijski, razvojni, invalidski in preživninski sklad Republike Slovenije
- Code Applications and Maintenance Program (CAMP); Thermal-Hydraulic Code Applications and Maintenance
- Dr. Andrej Prošek
- United States Nuclear Regulatory Commission, USNRC
- 6. Research of Conjugate Heat Transfer in Turbulent Pipe Flow
- Prof. Iztok Tiselj Electricite De France S.a.
- 7. Financing of project visits at the Slovenian higher education institutions pilot project

- dr. Mikuž Dr. Blaž Mikuž

- Thermocoax Sas
- Independent expert opinion of modification 1007-XI-L Dr. Mitja Uršič

Nuklearna Elektrarna Krško d. o. o.

 Safety characteristics and severe accident management in selected nuclear power plants Dr. Matjaž Leskovar

GEN energija, d.o.o.

### NEW CONTRACTS

1. Cooperation in an international CAMP and CSARP program

## VISITORS FROM ABROAD

- Prof. dr. Masaki Saito, Tokyo Institute of Technology (Tokyo, Japan), 16.-17. January 2018
- Dr Taka Fukuzaki, Tokyo Institute of Technology (Tokyo, Japan), 16.-17. January 2018
   Dr. Sofiane Benhamadouche, Electricité de France (EDF) Research and Development
- (Chatou, France), 22.-23. March 2018

## STAFF

#### Researchers

- 1. Prof. Leon Cizelj, Head
- 2. Dr. Martin Draksler
- 3. Dr. Samir El Shawish
- 4. Asst. Prof. Ivo Kljenak
- 5. Dr. Boštjan Končar
- 6. Dr. Matjaž Leskovar
- 7. Asst. Prof. Marko Matkovič
- 8. Dr. Blaž Mikuž
- 9. Dr. Andrej Prošek 10. Prof. Iztok Tiselj
- Prof. IZtok Tisel
   Dr. Mitia Unitia
- 11. Dr. Mitja Uršič
- 12. Dr. Andrija Volkanovski
- Postdoctoral associates 13 Dr Oriol Costa Garrido
- 14. Dr. Cedric Cyril Henri Flageul, left 01.08.18

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- Dr. Andrej Prošek Nuklearna Elektrarna Krško d. o. o. Joint Expert Assessment of the Outa
- Joint Expert Assessment of the Outage Activities, Interventions and Tests during a shutdown and refueling outage 2018 Dr. Mitja Uršič Elektroinštitut Milan Vidmar
- Analysis of Krško NPP Safety Upgrade Influence on Severe Accident Management Guidelines with MELCOR 2.2 Dr. Matjaž Leskovar
- Ministry of the Environment and Spatial Planning
- Investigation of turbulent heat transfer in an annulus throughadvanced experimental and computational methods
  - Prof. Iztok Tiselj Nuklearna Elektrarna Krško d. o. o.
- Dr Martin Ferrand, Electricité de France (EDF) Research and Development (Chatou, France), 22.-23. March 2018
- 5. Dr Bojan Ničeno, Paul Scherrer Institute (Villigen, Switzerland), 9.-13. April 2018
- 6. Prof. Hiroshige Kikura, Tokyo Institute of Technology (Tokyo, Japan), 11. July 2018
- Mr Anil Kumar Basavaraj, University of Rostock (Rostock, Germany), 7. May 2018-30. April 2019

#### Postgraduates

- 15. Tadej Holler, M. Sc. (B)
- 16. Janez Kokalj, M. Sc. (B) 17. Rok Krpan, M. Sc. (B)
- 17. Rok Krpan, M. Sc. (B) 18. Matic Kunšek, M. Sc. (B)
- 19. Jure Oder, M. Sc. (B)
- 20. Dr. Matej Tekavčič
- 21. Boštjan Zajec, M. Sc. (B)
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- 22. Sandi Cimerman, B. Sc.
- 23. Andrej Sušnik, B. Sc.
- Technical and administrative staff
- 24. Tanja Klopčič
- 25. Zoran Petrič, M. Sc. (B)
- 26. Nina Rehar, M. Sc. (B)
- Tadej Holler, Ed. M. J. Komen, Ivo Kljenak, "Hydrogen-air-steam deflagration experiment simulated using different turbulent flamespeed closure models", *Journal of nuclear engineering and radiation science*, 2018, 4, 3, 031009.
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- 2. Houjun Gong, Ying Wang, Yuanfeng Zan, Pengzhou Li, Ivo Kljenak, Etienne Studer, Ahmed Bentaib, Namane Mechitoua, "Experiment on light gas layer erosion in small-scale MCTHBF containment experimental facility", In: 12th International Topical Meeting on Nuclear Reactor Thermal-Hydraulics, Operation and Safety, (NUTHOS-12), Qingdao, China, October 14-18, 2018, 2018.
- 3. Andrej Prošek, "Status of CAMP activities in Slovenia", In: 2018 Fall CAMP meeting: December 11-13, Rockville, MD, USA, 2018.
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- 15. Jure Oder, Iztok Tiselj, "Direct numerical simulations of thermal fluctuations in a flow over a backward facing step with solid walls", In:

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- 28. Boštjan Končar, Jernej Kovačič, Martin Draksler, B. Schneider, "Thermal analysis of MST probe exposed to fusion relevant SOL plasma", In: Igor Jenčič (ed.), *Proceedings*, 27th International Conference Nuclear Energy for New Europe - NENE 2018, Portorož, Slovenia, September 10-13, 2018, 604.
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- 37. Rok Krpan, Ivo Kljenak, "Porazdelitev lahkega plina v eksperimentalni napravi zadrževalnega hrama", In: Klemen Ambrožič (ed.), et al., Zbornik 5. konference mladih jedrskih strokovnjakov: povzetki prispevkov, predstavljenih na konferenci v Reaktorskem centru Podgorica, 26. 2. 2018, 2018, 29.

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## INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

- Boštjan Končar, Andrej Prošek, Matjaž Leskovar, "Surrogate model applied for analysis of uncertain parameters in turbulent mixing flows", In: Adela Ionescu (ed.), *Computational fluid dynamics: basic instruments and applications in science*, 2018, 377-396.
- 2. Boštjan Končar, Luka Klobučar, "Use of CFD codes for calculation of radiation heat transfer", In: Konstantin Volkov (ed.), *Heat transfer: models, methods and applications*, 2018, 23-41.
- 3. Iztok Tiselj, "Penetration of turbulent temperature fluctuations into the heated wall", In: Gennady Ziskind (ed.), George Yadigaroglu (ed.), *Multiphase flow phenomena and applications: memorial volume in honor of Gad Hetsroni*, 2018, 51-66.

#### PROFESSIONAL MONOGRAPH

 Andrej Prošek, RELAP5 and TRACE Simulation of Hot Leg Break LOCA Experiment on LSTF, Washington: U.S. Nuclear Regulatory Commission, 2018, NUREG/IA – 0494.

#### MENTORING

1. Matej Tekavčič, *Modelling of isothermal separated gas-liquid flow in a vertical pipe:* doctoral dissertation, Ljubljana, 2018 (mentor Ivo Kljenak; co-mentor Boštjan Končar).

## 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, education and training, and 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, for both research and applicative projects. In addition, it is used for performing regular radiological measurements of radioactive waste and irradiated samples.

Members of the reactor staff operate and maintain the reactor. They also participate in other activities, requiring specialists skilled in working with sources of radiation and in reactor technology, such as the servicing of industrial radioactive sources and the surveillance of fuel management in NPP Krško.

am that is approved on a weekly basis by the Heads of the

The reactor operated in accordance with the program that is approved on a weekly basis by the Heads of the Head: RIC and the Radiation Protection Unit – RPU (SVPIS in Slovene). In 2018, the reactor operated for 143 days and **Prof. Borut Smodiš** 

produced 116.0 MWh of heat. Altogether twenty-seven pulses were carried out and 1019 samples were irradiated in the rotary specimen rack, irradiation channels and 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 irradiated radioactive samples.

In 2018, the reactor was mainly used as a neutron source for neutronactivation analysis, the irradiation of electronic components, education and training. For educational purposes, it was mostly used by the J. Stefan Institute's Nuclear Training Centre. For the irradiation of samples, it was mostly used by the Department of Environmental Sciences – O2 and the Department of Experimental Particle Physics – F9. The Reactor Physics Department – F8 used the reactor for experiments in reactor physics.

The shutdown reactor, being a powerful source of gamma radiation, was used for testing the resistance of electronic components to radiation, the irradiation of ceramic samples for the Department of Electronic Ceramics (K5) and the sterilization of samples for the Department for Nanostructured Materials (K7).

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

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.;



Figure 1: In 2018, our team of researchers and operators has successfully calibrated self-powered neutron detectors for the French company Themrocoax.



Figure 2: Pulse-mode operation by our former operator Karl Svetek, who was part of the first team of JSI TRIGA operators.





Figure 3: A group of researchers from the University of Lancaster is designing an underwater ROV, which will investigate the interior of damaged reactors in Fukushima. Radiation-hardness tests were performed at the JSI TRIGA reactor.



Figure 4: Underwater ROV that will investigate the interior of the damaged reactor in Fukushima.



Figure 5: Hot-Cell facility is used to prepare radioactive waste for longterm storage.

- Verification and validation of methods for calculating the transport of neutrons, photons and electrons;
- Development of educational tools in reactor physics.

In the framework of a collaboration between the Reactor Physics Department (F8) and the French Alternative Energies and Atomic Energy Commission (CEA), Cadarache, the following activities were carried out:

- SLO-CEA project BI-FR/CEA/16-18/001: Experimental 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;
- Experimental Testing of Self-Powered Neutron Detector Assemblies for CEA DISCOMS Project;
- Experimental Testing of Self-Powered Neutron Detector Assemblies for CEA INFINI Project;
- Design of irradiation device for FT-TIMS method at the JSI TRIGA Mark II Reactor: Irradiation of FT-TIMS samples.

Due to good formal and informal cooperation with CEA, the above activities will be continued in 2019.

In January, developers of a submarine robot from the University of Lancaster were hosted. The robot will investigate the damaged reactors in Fukushima and must therefore be sufficiently resistant to radiation. Resistance testing was carried out at the JSI TRIGA Reactor.

In the first third of the year, glycol and glycerine samples were irradiated with gamma rays and neutrons for the University of Lancaster. The results were published in Proceedings of the  $27^{\text{th}}$  International Conference "Nuclear Energy for a New Europe" (NENE2018), which took place from 10 to 13 September 2018 in Portorož, Slovenia.

The JSI TRIGA Mark II Reactor is a reference centre for neutron irradiation in the development of ATLAS detectors (http://aida2020.web.cern.ch/ content/jsi) in CERN. Since 2011, the TRIGA Reactor has participated in the FP7 AIDA (*Advanced Infrastructures for Detectors and Accelerators*) and in the project "*Horizon 2020-the AIDA-2020 GA No. 654168, Task 15.5-Irradiation Facilities*" (*http://aida.web.cern.ch/aida/index.html*), which brings together advanced European infrastructures for future particle-physics experiments. This cooperation continues as part of the AIDA II project.

In the scope of the NATO SPS project E-SiCure (http://e-sicure.web. ua.pt/), in which the Reactor Physics Department (F8) is also involved, the reactor was used to perform test irradiations of silicon-carbide samples to study the neutron-induced defects in the material. The project is aimed at engineering silicon carbide material for the detectors of special nuclear material for border and port security.

In cooperation with the Institute of Metals and Technology, Ljubljana (IMT), the irradiation of material intended for the medical production of artificial hips has started. The aim is to improve the integration between the molecules and make the material more resistant to abrasion by gamma rays irradiation.

In March, a group of students from the Massachusetts Institute of Technology (MIT) was hosted for a one-week course of practical exercises in reactor physics.

In October, RIC hosted the *"Safety evaluation, licensing and oversight of research reactors"* course, in the framework of the EC's program INSC (Instrument for Nuclear Safety Cooperation). The attendees performed practical exercises at the JSI TRIGA Mark II reactor. After the course, two participants continued their training for an additional 6 weeks.

In November, the demanding experimental testing of self-powered neutron detectors for the Thermocoax company was performed.

Cooperation with Slovenian companies DITO d.o.o. and Nanocut d.o.o. in the development of radiation-resistant LED lights has continued

In the framework of training and education, different lectures and practical exercises were conducted at the reactor. The participants were students from Slovenian universities: the Faculty of Mathematics and Physics, Ljubljana (Programme: Master of Science in Nuclear Engineering Course: Experimental reactor physics), the Faculty of Electrical Engineering, Ljubljana; and the Faculty of Energy Technology, Maribor. To carry out the exercises, the reactor was used for about 3 months, and the average number of participants per experiment was 10. All the exercises were performed by the RIC personnel in collaboration with the Reactor Physics Department (F8).

In 2018, there were more than 60 group visits to the reactor. The visitors were mainly foreign scientists, students and 48 groups of schoolchildren. Their total number was more than 1800. In March, the *Jožef Stefan Institute's Open Days* were organized, when the reactor was visited by around 250 people.

## INTERNATIONAL PROJECTS

- 1. Training Fee for IAEA Fellow Mr. Esserhir El Fassi Prof. Borut Smodiš
- IAEA International Atomic Energy Agency
   Training Costs for IAEA"s Fellow Mr. Ismail Marrhich (FS-MOR1011-1802851), 2.9.-28.9.2018
  - Prof. Borut Smodiš
  - IAEA International Atomic Energy Agency
- Training Costs for IAEA"s Fellow Mr. Said Ótmani (FS-MOR1011-1802851), 2.9.-28.9.2018 Prof Borut Smodiš
  - IAEA International Atomic Energy Agency

## R & D GRANTS AND CONTRACTS

- Irradiation for FT-TIMS Method at the JSI TRIGA Mark II Reactor Prof. Luka Snoj
- Irradiations in TRIGA Nuclear Reactor
- Prof. Borut Smodiš 3. Experimental Testing of Self-Powered Neutron Detector Assembly for CEA DISCOMS Project

## VISITORS FROM ABROAD

- 1. Loic Barbot, Hamid Makil, Stéphane Fourrez, CEA Cadarache, St Paul lez Durance Cedex, France, 15 January 2018 – 19 January 2018
- Kamada So, Kato Michio and Nishimura Kazuyo, National Institute of Maritime Port and Aviation Technology, Tokyo, Japan; dr. Ashley Jones, prof. dr. Malcolm Joyce and Arran Plant, Lancaster University, United Kingdom; Matthew J. Nancekievill and Watson Simon, University of Manchester, United Kingdom; Keisuke Okumura, Japan Atomic Energy Agency (JAEA), Japan; Katakura Junichi, Nagaoka University of Technology, Japan; So Kamada and Michio Kato, National Maritime Research Institute, Japan; Kazuya Nishimura, Tokyo Institute of Technology, Japan; 6 February 2018 – 8 February 2018
- Georgi Gorine and Giuseppe Pezzulo, CERN, Świtzerland, 5 March 2018 9 March 2018
   Ivana Capan, Zoran Ereš and Tomislav Brodar, Institut Ruđer Bošković, Croatia; Takeshi
- 4. Vana čapani, zorah Eres and Fornstav Brodar, institut Ruder Dosković, Orada, rakesin Ohshima, National Institutes for Quantum and Radiological Science and Technology, Japan; Yuichi Yamazaki, MSC Software Corporation, Japan; José Coutinho, Universidade de Lisboa, Portugal; Željko Pastuović and Adam Sarbutt, Australian Nuclear Science and Technology Organisation (ANSTO), Australia; 28 May 2018 – 30 May 2018
- Ismail Marrhich and Said Otmani, Centre National de l'Energie des Sciences et de Techniques Nucléaires (CNESTEN), Rabat, Morocco, 3 September 2018 -28 September 2018

## STAFF

Researcher 1. Prof. Borut Smodiš, Head

- Postgraduate
- 2. Anže Jazbec, B. Sc.

Technical and administrative staff

3. Andrej Gyergyek, B. Sc.

Figure 6: Maintenance on the pneumatic transfer system inside the Hot Cell.

Prof. Borut Smodiš

- Cea List Institute, Dept. Of Metrology, 4. Irradiation and Analysis of Nano SiC Samples in the Year 2017 Anže Jazbec, B. Sc.
- National Nuclear Research Center 5. Gamma and Neutron Irradiation of Submersible ROV
- Anže Jazbec, B. Sc. Lancaster University 6. Irradiation of Glycol
- Anže Jazbec, B. Sc. Lancaster University
- 7. Irradiations on the TRIGA Reactor Prof. Borut Smodiš
- Experimental Testing of Self-Powered Neutron Detector Assemblies for CEA INFINI Project
- Prof. Borut Smodiš Cea List Institute, Dept. Of Metrology,
- Experimental Testing of Self-Powered Neutron Detectors for the Thermocoax Company Prof. Borut Smodiš Thermocoax Sas
- Irradiation of FT-TIMS Samples
   Anže Jazbec, B. Sc.
   Comparison of A. L. Energie A. L. Ener
  - Cea Commissariat A L' Energie Atomique
- 6. Dr. John E. Kelly, American Nuclear Society (ANS), President, 7 September 2018
- Loic Barbot, Alexandre Dabat Blondeau, Moline Yoann, CEA, France, 26 September 2018 - 27 September 2018
- dr. Elchin Huseynov, National Nuclear Research Center, Baku, Azerbaijan, 7 October 2018 – 21 October 2018
- Loic Barbot and Damien Fourmentel, CEA, France; Jasper Heiko, Framatome, Germany; 8 October 2018 – 19 October 2018
- Tetiana Vorontsova, State Nuclear Regulatory Inspectorate of Ukraine, Kiev, Ukraine; Firdavs Salomov, Nuclear and Radiation Safety Agency of Tajikistan, Dushanbe, Tajikistan; 8 October 2018 – 16 November 2018
- 11. Rudy Ferraro in Gabriele Piscopo, CERN, Genève, Switzerland, 24 25 October 2018
- Georges Helleux, Vincent Salou, Laurent Pichon, Thermocoax, France; Li Cai, Yunfeng Lv, Dongsheng Li, China Nuclear Power Technology Research Institute, China; Loic Barbot, CEA, France; Ludo Vermeeren, SCK • CEN, Belgium; 19 November 2018 – 30 November 2018
- 13. Loic Barbot, Hassen Hamrita, Gregoire De Izarra, Mathieu Trocme, CEA, France, 5 December 2018 6 December 2018
- 14. Hubert Carcreff, Nicolas Thiollay, CEA, France, 9 December 2018 21 December 2018
- 4. Marko Rosman
- 5. Sebastjan Rupnik, B. Sc.
- 6. Nina Udir, B. Sc.
- 7. Andraž Verdir, B. Sc

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#### **ORIGINAL ARTICLE**

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- 3. Anže Jazbec, Sebastjan Rupnik, Vladimir Radulović, Klemen Ambrožič, Borut Smodiš, Luka Snoj, "The Jožef Stefan Institute TRIGA research reactor activities in the years 2017 and 2018", In: Igor Jenčič (ed.), *Proceedings*, 27th International Conference Nuclear Energy for New Europe - NENE 2018, Portorož, Slovenia, September 10-13, Ljubljana: Nuclear Society of Slovenia, 2018.
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#### MONOGRAPH

1. Sebastjan Rupnik, Borut Smodiš, "Automation of a pneumatic transport system for neutron activation analysis", In: N. P. Barradas, *Development* of an integrated approach to routine automation of neutron activation analysis: results of a coordinated research project, (IAEA TECDOC series **1839**) 2018, 170-179.

## 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 of 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 primary mission is to maintain the computing networks, services and hardware necessary to support the work of users at the Jožef Stefan Institute, their collaborators, projects and research groups. We provide a high level of connectivity 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. NIC is responsible for four main domains: networking infrastructure, network security, network services and distributed network supercomputing.



Networking Infrastructure. The Networking Infrastructure Centre is responsible for the development, man-Head: agement, administration and support of the Institute's physical networking infrastructure. It delivers support for Dr. Jan Jona Javoršek local networks, ensuring local and internet connectivity for users and services at the Institute. This task includes the management of wireless networks at all Institute locations and providing 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, connections to scientific VPN networks through GÉANT etc.).

Physical Network: In 2018 we extended and optimised parts of the physical network and cabling installations and continued upgrading our active equipment, including wireless access point installations and core backbone network routers, to support extensions and optimisations of the Institute's backbone network. The connectivity between the Reactor Centre Podgorica and the Jamova campus has been improved and the two networks have been integrated. We supported advancing use of virtual network links for dispersed internal networks, (super)computing clusters and virtual machine farms, including a new approach for remote VPN access and device support access for outside contractors. External connections have been maintained and optimised to support high network throughput work and experiments needed for the collaboration within WLCG (Worldwide Large Hadron Collider Computing Grid) for ATLAS, but also Belle2 and other EGI and PRACE using projects over general GÉANT networks and also dedicated scientific VPNs, such as LHCONE and PRACE.

Monitoring: Development and integration of our traffic, event and status-monitoring infrastructure, implemented on the basis of software packages Nagios for monitoring and alerting, Ganglia, Cacati and

A modern up-to-date multiple 10 Gbit/s network backbone supporting modern protocol stacks and dedicated external links is the basis of a flexible modern network environment at the Jožef Stefan Institute, where high availability and advanced services supporting many fixed and wireless clients is a requirement for day-to-day work.

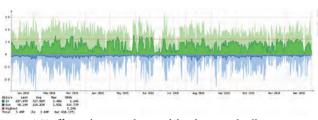


Figure 1: Traffic on the general network has been gradually increasing throughout 2018 while the amount of traffic with dedicated science VPNs has been limited by available national connectivity.

Observium for network monitoring, a customised dynamic analytical visualisation package built with Kibana and ElasticSearch, and Grafana-based aggregated monitoring to display an integrated report and 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: Due to the introduction of cheaper components and better central control we were able to continue to improve the wireless coverage and density of our wireless networks to alleviate the effect of increasing numbers of users and devices and their more frequent and more critical usage patterns.

Network Security. The NIC is responsible for implementing security measures and policies at the external network borderline, in the internal network and regarding the services and software deployments for the users. External network security is implemented with the dynamic management and configuration of active deep-packetinspection firewall systems and routing configurations, while dedicated links are managed with passive measures (configuration, filtering and supervision) to facilitate high throughput. Constant dynamic supervision, traffic monitoring and event analysis is needed to ensure suitable security in the complex constraints and requirements of an open academic network that collide with current security considerations and demands for high throughput.

Internal development of e-mail security and dynamic network firewalling, encrypted connections, virtual networks, advanced analysis and monitoring ensure the security of an open academic network in the age of a hostile Internet. Ensuring a secure and open environment requires disproportionate increases in equipment capabilities and efforts in the dynamic security-policy configuration, event monitoring and analytics. Due to increasing threats from the outside network we have been restricting our security measures at the network perimeter and maintaining a stricter auditing policy of existing e-mail, eduGAIN/AAI and Eduroam accounts.

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 SI-CERT, 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

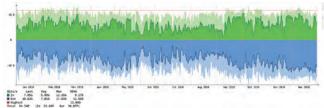
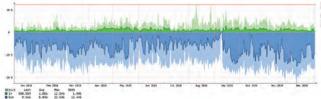


Figure 2: Traffic on the 20G bit/s dedicated science VPN LHCOne link between the Institute and Arnes is limited by national connectivity. While generally slowly increasing, it fluctuates wildly due to differences in loads from CPU-limited and data-limited computing tasks.



28 598,501 1,685 12,560 1,990 Out 9,505 8,945 22,536 12,445 BigBent 12,465 Total 31,73# (34 4,28# 0ut 27,449)

Figure 3: Internal 40G bit/s link connecting Jamova campus with the JSI computing centre Teslova allows efficient usage of the computing and data infrastructure in the centre.

distributed computing network consortium SLING. The national science certificate agency SiGNET CA (Slovenian Grid Network Certification Authority), managed by the NIC, is a full member of EU Grid PMA (EU Grid Policy Management Authority) and IGTF (Interoperable Global Trust Federation). We participate in the work of the Slovenian network technology and security association SINOG (Slovenian Network Operators Group) and supported the organization by hosting a technical workshop 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 the in-house software development of Amavisd, the open-source e-mail content filter, and its SpamAssassin package integration, but also with continuous improvements in the support for new and advanced features in e-mail message and protocol stack handling and filtering.

*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. We have also continued expanding the use of TLS encryption by widely introducing "Let's Encrypt" certificates to many services. The number or users of our VPN infrastructure has been steadily increasing.

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 in support of certain core or

The constant growth of network services and network computing with ever better support for collaboration and teamwork, software development, data protection and access to large computing and data resources for scientific research at home and abroad are a crucial cornerstone for modern scientific work. 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 made up of services supporting our users (calendaring, event management, directories) and software/system developers (code repositories, integration and verification, licence management, mobile platform software development, integration and shipping for Apple Appstore and Google Play). The

software-development repository has stood out by attracting a large number or new users in recent years, and in 2018 our testing deployment of a NextCloud file repository has gained a large number of users as well. We also provide physical server hosting and management, aimed primarily at larger projects and systems, the administra-

tion 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 2018, we have continued expanding the computationally intensive infrastructure in the new computing centre at Teslova that was established in 2015, while at the NIC computing centre, where we can provide highly

reliable cooling, network connectivity and uninterrupted power supply for critical services, we have continued to host ever more computationally less-intensive servers from several departments. We have also expanded our web-hosting activity (over 90 distinct virtual servers).

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 now used extensively since it gives our users easier access to numerous national and international services using their institute credentials. We hope that this facility will simplify user and authentication management at the Institute and for software developers who work on internal projects and services in the future.

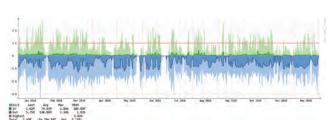


Figure 4: Network usage at the common cluster reflects large differences in the data sets and network requirements that we see due to very different user requirements.

Network super-computing. In the field of network computing technology and infrastructure, high-throughput computing, high-performance computing, network and grid middleware, vectorisation, software containers, virtualisation and ICT as a service (cloud) continued to converge, which confirmed our strategy of integrating all of the above approaches. The NIC has continued to maintain central computing facilities for the JSI and has been collaborating with our other computing clusters, while taking part directly in the Slovenian National Supercomputing Network SLING as a funding member and core partner, participating in the development and integration efforts of the consortium. 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 2018, the New System Cluster (NSC), the common computing cluster in the new facilities of the Jožef Stefan Institute's Computing Centre Teslova, has continued to see a steady increase of user demand. The 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 important for the promotion and availability of supercomputing at

the Jožef Stefan Institute, since it is the only cluster that is available to all researchers at the Institute and can therefore provide 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, besides supporting users of JSI clusters, we also work on the integration of clusters with the national supercomputing network SLING using the NorduGrid ARC Grid Middleware to enable users to use all the resources in the network with the same interfaces and to use software containers to facilitate portability of user software.



Figure 5: Power consumption of the JSI computer centre Teslova reflects how much the facility is used. There is a short drop at the end of June due to an unscheduled cooling-system maintenance caused by power fluctuation. The graph shows higher efficiency of the cooling system in the winter months, when the air is sufficiently cool to use free cooling.

In the domain of network supercomputing we have been most involved with the Slovenian National Supercomputing Network (SLING), but we also worked within the European Grid Initiative EGI (with development of the EGI Federated Cloud pilot – federated infrastructure as a service), PRACE (Partnership for Advanced Computing in Europe), the NorduGrid ARC collaboration and a number of international projects (ATLAS – dedicated link, Belle2 – computing support, CLARIN – support for different services of Slovenian national node, ELIXIR – collaboration with the national node and the European collaboration). SLING has supported a number or research projects and applications, among others in high-energy physics, medical sensor and image analysis, theoretical physics, astrophysics, biochemistry, protein-folding simulations, crystal analysis, knowledge technologies, artificial intelligence, 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. Members of NIC have also contributed as advisors in EuroHPC and European Open Science Cloud.



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   Barbara Krašovec, M. Sc.
   Mark Martinec, B. Sc.

- Technical and administrative staff 5. Ivan Ivanjko 6. Janez Jezeršek 7. Matjaž Levstek 8. Janez Srakar 9. Matej Wedam

## 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, IEEExplore 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.



Dr. Luka Šušteršič

### INTERNATIONAL PROJECT

1. Sales of Scientific Publication Dr. Luka Šušteršič

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- Technical officers
- 1. Dr. Luka Šušteršič, Head
- 2. Marjan Verč, M. Sc. Technical and administrative staff
- Suzi Korošec, B. Sc.
- Jasna Malalan

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

- 1. Purchase and Sale of the Book Advances in Robot Kinematics 2016 Dr. Luka Šušteršič
- 5. Katarina Modic, B. Sc.
- 6. Alenka Ana Stante, B. Sc.
- Jože Škulj
   Branka Štrat
- Branka Štrancar
   Ana Tratnik
- 10. 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 (GHGs) 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 emission trading. Nevertheless, it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as also being increasingly involved in European research projects.



#### Energy and the environment

In 2018, the EEC, with its professional work, ensured high-quality support to ministries in the preparation of Head: the strategic development documents and transfer of EU legislation. Energy efficiency is a priority field to achieve Stane Merše, M. Sc. global climate and energy goals and in accordance with the Directive on Energy Efficiency (2012/27/EU) the EEC report on the implementation of the Action Plan for Energy Efficiency for the period 2014-2020 was prepared. The EEC also cooperated in the updating of the Action Plan for Renewable Energy Sources for the period 2010-2020 and started with preparation of the analytical basis for the National Energy and Climate Plan (NECP) of Slovenia.

Within the expert support of the Ministry of the Environment and Spatial Planning the EEC's activities focused on the preparation of the analytical basis and the long-term GHG emission projection within the LIFE ClimatPath2050

project with the goal being to contribute to better climate governance by enhanced monitoring and planning of the GHG mitigation measures in buildings, transport, industry, agriculture, forestry and waste. The first Climate Action Mirror was prepared, which also presents a report on the implementation of the Operative Programme of Measures for GHG emission reduction until 2020 and the Local Climate Activity Scoreboard of Municipalities (Figure 1). The EEC was involved in the preparation of the analytical basis for international reporting in the framework of the MMR and the preparation of the Third Biennial Report from Slovenia under the mechanism of the UNFCCC. With the start of the preparation of the Action Plan, the EEC continued its professional support for the design of goals and national policy concerning pollutants from the NEC directive.

The EEC cooperates with the Statistical Office of the Republic of Slovenia, where every year it prepares a model calculation for fuels and energy use in households for the national energy statistics. Also in 2018, the EEC continued with activities of the state referential centre for energy with the preparation of an expanded set of indicators for energy and the environment. For the Energy Agency the EEC set new reference electricity generation costs for the support scheme for RES and cogeneration electricity production units.

#### Promotion of efficient energy use and energy consulting

In 2018 the EEC continued with its training activities where already the eleventh cycle of energy-managers training was successfully concluded within the European programme EUREM. Due to the very positive reactions of the participants and their interest (in Slovenia there are already more than 225 energy managers with the 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.

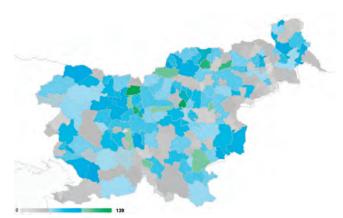


Figure 1: Local Climate Activity Scoreboard of Municipalities - The value of stimulated investments in energy efficiency and renewable energy in households per capita in 2018.

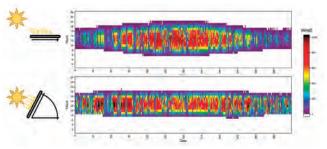


Figure 2: Analysis of solar radiation during a year on the horizontal (top) and suitable leaning surface (bottom).



Figure 3: Awarding of prizes to the 11th generation of EUREM energy managers.

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.

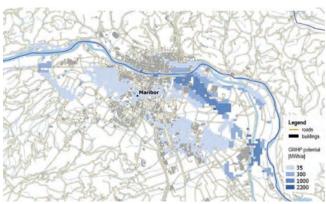


Figure 4: Assessment of the shallow geothermal energy potential for ground-water heat-pump systems for that area of the City of Maribor



*Figure 5: First Study visit on Energy Performance Contracting (EPC) in Slovenia. within the CA-EED project.* 

An intensive development of the GIS tool for the spatial analysis of heat consumption in buildings ("heatmap") continued with an upgrade and update of the heat-map application for the City of Maribor and implemented a detailed spatial analysis of the shallow geothermal potential of Slovenia (Figure 4).

In 2018 the EEC carried out deep energy audits in the companies Ljubljanske mlekarne, BTC Sberbank and Telekom. The professional cooperation with Luka Koper continued with energy audits of the port terminals and a study of the technical potential for powering ships while they are berthed in the port and cooperation with the steel company Metal Ravne in the field of waste-heat utilisation. For the Motorway Company in the Republic of Slovenia (DARS) there was an elaboration of a study of the methodology for the evaluation of  $CO_2$  emissions and other air pollutants from vehicles on motorways in Slovenia.

The EEC prepared the programme for the 20<sup>th</sup> 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 2018 the EEC carried out as many as 10 international projects, financed from the European Union resources in the framework of LIFE and HORIZON 2020. The projects cover activities in the fields of:

- Slovenian mid-century climate path (LIFE ClimatePath2050)
- Heat-pipe technology for waste-heat recovery in industry (ETEKINA),
- Driving investment in energy-efficiency services through quality assurance (QualitEE),
- Promotion of the introduction of energy contracting in the public and private sectors in the EU (guarantEE),
- Energy contracting Plus Plus (EPC Plus),
- Tool for the evaluation of the suitability of integrated energy retrofit (Enerfund),
- Monitoring of indicators for energy use and energy efficiency in the EU (ODYSSEE MURE),
- Improving the Performance of District Heating Systems in Central and Eastern Europe (KeepWarm)
- carrying out the EU directive on energy efficiency (CA EED),
- carrying out the EU directive on renewable energy sources (CA RES).

Projects include cooperations with R&D organisations from Europe with a strong emphasis on concrete applications and the promotion of energy efficiency. In the framework of each project the EEC staff took part in numerous foreign professional meetings and visits.

## Some outstanding achievements in the past three years

- 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 **Transparense** 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), also supported 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.

#### Organization of conferences, congresses and meetings

- 1<sup>st</sup> Supervisory Meeting on Life project ClimatePath2050, Jožef Stefan Institute, Reactor Centre Podgorica, 18<sup>th</sup> January, 2018;
- 2. Presentation of the existing GHG projections, shaping criteria for scenario comparison, workshop at EU project Life ClimatePath2050, Jožef Stefan Institute, Reactor Centre Podgorica, 7th February, 2018;
- European Energy Manager, 11th group, training, Jožef Stefan Institute, Reactor Centre Podgorica, 14<sup>th</sup>-16<sup>th</sup> February, 14<sup>th</sup>-16<sup>th</sup> March, 18<sup>th</sup>-20<sup>th</sup> April, 15<sup>th</sup> -18<sup>th</sup> May; conclusion on 11<sup>th</sup> December, 2018;
- Prospective of energy contracting and financing renovation of buildings in Slovenia in period 2020-2030, consultation at EU project Life ClimatePath2050 and EPC+, Ljubljana, Chamber of Commerce and Industry of Slovenia GZS, 27<sup>th</sup> February, 2018;
- Emissions in agricultural sector current status, calculations and factors, workshop at EU project Life ClimatePath2050, Ministry of Agriculture, Forestry and Food MKGP, Ljubljana, 15th March, 2018;
- 6. Preparation workshop for Climate Action Mirror 2018 workshop at EU project Life ClimatePath2050, Slovenian environment agency ARSO, Ljubljana, 27<sup>th</sup> March, 2018;
- 7. 21<sup>st</sup> Energy Managers Days, Portorož, 16<sup>th</sup> and 17<sup>th</sup> April, 2018;
- 8. Climate Action Mirror 2018, European Union House, Ljubljana, 17<sup>th</sup> April, 2018;
- 9. Financial and planning district heating systems, workshop at EU project Life ClimatePath2050, Slovenian environment agency ARSO, Ljubljana, 11<sup>th</sup> May, 2018;
- Energy poverty, workshop at EU project Life ClimatePath2050, Slovenian environment agency ARSO, Ljubljana, 17<sup>th</sup> May, 2018;
- 11. How successful is Slovenia with implementing energy efficiency measures (ODYSEE-MURE), lecture at EU project Life ClimatePath2050, Jožef Stefan Institute, Reactor Centre Podgorica, 22<sup>nd</sup> May, 2018;
- Potentials for reducing GHG emission in e-mobility, workshop at EU project Life ClimatePath2050, Jožef Stefan Institute, Reactor Centre Podgorica, 29th May, 2018;
- 13. GDP projections, workshop at EU project Life ClimatePath2050, Institute for Economic Research IER, Ljubljana, 31<sup>st</sup> May, 2018;
- 14. Award ceremony on the photo contest »Climate Path« at EU project Life ClimatePath2050, Jožef Stefan Institute, Ljubljana, 18<sup>th</sup> June, 2018;
- 15. Potentials of shallow geothermal energy, Geological survey of Slovenia GeoZS, Ljubljana, 19th June, 2018;
- Energy prices projections, workshop on EU project Life ClimatePath2050, Slovenian environment agency ARSO, Ljubljana, 21<sup>st</sup> June, 2018;
- 17. Planning, financing and implementation of climate measures in municipalities launch of Local scoreboard 2018 at EU project Life ClimatePath2050, European Union House, Ljubljana, 5<sup>th</sup> October, 2018;
- 18. Preparation of Long term climate strategy for low emission scoping at EU project Life ClimatePath2050, Slovenian environment agency ARSO, Ljubljana, 6<sup>th</sup> November, 2018;
- Heat pipe technology for thermal energy recovery in industrial applications, 2nd Steering Committee on the EU project ETEKINA, Jožef Stefan Institute, Reactor Centre Podgorica, 17<sup>th</sup>-19<sup>th</sup> September, 2018;
- 20. CA EED study visit, Jožef Stefan Institute, Reactor Centre Podgorica, 8th-9th November, 2018;
- 21. Projections of Transport Work at EU project Life ClimatePath2050, Jožef Stefan Institute, Reactor Centre Podgorica, 21<sup>st</sup> November, 2018;
- 22. Preparation of Climate mirror working gathering at EU project Life ClimatePath2050, National Museum of Slovenia, Ljubljana, 23<sup>th</sup> November, 2018;
- 23. New approaches to implementation of energy efficiency projects and challenges of energy services contracting; Training in the framework of QualitEE, GuarantEE and ENERFUND (EU H2020) projects, Jožef Stefan Institute, Reactor Centre Podgorica, 5<sup>th</sup> December, 2018.

## INTERNATIONAL PROJECTS

- 1. "LIFE ClimatePath 2050" Slovenian Path towards the Mid-Century Climate Target Andreja Urbančič, M. Sc.
- Borzen, d. o. o. 2. H2020 - EPC\_PLUS; Energy Performance Contracting Plus Damir Staničić. M. Sc.
- European Commission 3. H2020 - ENERFUND; An ENErgy Retroit FUNding rating tool Jure Čižman, M. Sc.
- European Commission
- 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 Staničić, M. Sc. European Commission
- Halopean commission frameworks for Energy Efficiency Services to scale up Responsible Investment in the Building Sector Damir Staničić, M. Sc.
- European Commission
- H2020 KeepWarm; Improving the performance of district heating systems in Central and East Europe Stane Merše, M. Sc.
- European Commission
- RESEARCH PROGRAM
- 1. Modelling and environmental impact assessment of processes and energy technologies Dr. Fouad Al-mansour

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

- 1. Social acceptability of territorial effects in RES scenarios Andreja Urbančič, M. Sc.
- Evaluation of greenhouse gasses mitigation measures in industry Dr. Matevž Pušnik
   Development and design of energy consuption monitoring by control
  - Development and design of energy consuption monitoring by connecting various databases Dr. Fouad Al-Mansour
- LIFE ClimatePath 2050: Slovenian Path towards the Mid-Century Climate Target Andreja Urbančič, M. Sc.
- Ministry of the Environment and Spatial Planning 5. Evaluation of greenhouse gasses mitigation measures in industry
- Evaluation of greenhouse gasses initigation measures in industry Dr. Matevž Pušnik
   Ministry of the Environment and Spatial Planning
- Ministry of the Environment and Spatial Planning 6. Development and design of energy consuption monitoring by connecting various databases
- Dr. Fouad Al-Mansour Ministry of Infrastructure

## NEW CONTRACTS

- 1. Cooperation in preparation of 7th National Communication and Slovenia's 3rd Biannual report according to UNFCC reporting provisions Matjaž Česen, B. Sc.
- Ministry of the Environment and Spatial Planning
- Concerted Action supporting the transposition and implementation of Directive 2009/28/EC (RES Directive) (CA-RES) Damir Staničić, M. Sc.
- Ministry of Infrastructure 3. Expert and technical support and the preparation of a proposal for a integrated National energy and climate plan Stane Merše, M. Sc. Ministry of Infrastructure

## VISITORS FROM ABROAD

- 1. Prof. dr. Hussam Jouhara, Brunel University, London, Great Britain, 1st 4th February, 2018
- 2. Iñigo Bonilla, University of the Basque Country, Bilbao, Spain, 30th November, 2018-1st March, 2019

### STAFF

- Researchers
- 1. Dr. Fouad Al-Mansour
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- 6. Matjaž Česen, B. Sc.
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- 9. Marija Kavčič, B. Sc.
- 10. Dr. Marko Kovač
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- 16. Marko Đorić, B. Sc.
- 17. Igor Ribič
- 18. Katarina Trstenjak, B. Sc.

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- 1. Boris Sučić, Goran Matešić, Boštjan Pavlič, Zvonko Košnjek, Stojan Petelin, "Evaluation of energy and environmental challenges od installing cold ironing case study Port of Koper", In: Marko Ban (ed.), *Digital proceedings*, 13th Conference on Sustainable Development of Energy, Water and Environment Systems, September 30 October 4, 2018, Palermo, Italy, 2018.
- Matevž Pušnik, Boris Sučić, Fouad Al-Mansour, Matjaž Česen, "Greenhouse gas mitigation policy and its impact on Slovenian industry", In: Marko Ban (ed.), *Digital proceedings*, 13th Conference on

Sustainable Development of Energy, Water and Environment Systems, September 30 - October 4, 2018, Palermo, Italy, 2018.

- 3. Gašper Stegnar, Tomo Cerovšek, "A progressive use of bim for energy renovation of office buildings: Establishing information requirements for decision-making in sustainability assessment", In: Abdul Ghani Olabi (ed.), Renewable and sustainable energy developments beyond 2030: proceedings of the 11th International Conference on Sustainable Energy & Environmental Protection, SEEP Conference 2018, 8-11 May 2018, Paisley, Scotland, 2018.
- 4. Gašper Stegnar, Matjaž Česen, Jure Čižman, Stane Merše, Damir Staničić, "Are the biomass boilers solutions for Slovenian households?", In: Abdul Ghani Olabi (ed.), Renewable and sustainable energy

developments beyond 2030: proceedings of the 11th International Conference on Sustainable Energy & Environmental Protection, SEEP Conference 2018, 8-11 May 2018, Paisley, Scotland, 2018.

- 5. Marko Kovač, Gašper Stegnar, Matjaž Česen, Stane Merše, "Assessing solar potential and battery instalment for self-sufficient buildings with simplified model", In: Abdul Ghani Olabi (ed.), Renewable and sustainable energy developments beyond 2030: proceedings of the 11th International Conference on Sustainable Energy & Environmental Protection, SEEP Conference 2018, 8-11 May 2018, Paisley, Scotland, 2018.
- 6. Blaž Luin, Stojan Petelin, Fouad Al-Mansour, "Microsimulation of electric vehicle energy consumption", In: Abdul Ghani Olabi (ed.),

Renewable and sustainable energy developments beyond 2030: proceedings of the 11th International Conference on Sustainable Energy & Environmental Protection, SEEP Conference 2018, 8-11 May 2018, Paisley, Scotland, 2018.

7. Marko Đorić, Andreja Urbančič, Polona Lah, Fouad Al-Mansour, Matevž Pušnik, Boris Sučić, Leon Cizelj, Andrija Volkanovski, "Policy and financial support Scheme for Renewable Energy Sources Utilization in Slovenia.", In: Abdul Ghani Olabi (ed.), Renewable and sustainable energy developments beyond 2030: proceedings of the 11th International Conference on Sustainable Energy & Environmental Protection, SEEP Conference 2018, 8-11 May 2018, Paisley, Scotland, 2018.

# 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 to other research institutions, universities and industrial partners. The equipment at the CEMM is used by researchers who are interested in the morphology and structural and chemical characterization of materials between the micrometre and the atomic levels. At the CEMM there are three scanning electron microscopes (SEM) JSM-5800, JXA-840A, JSM-7600F, two transmission electron microscopes (TEM) JEM-2100 (CO NIN) and JEM-2010F, and the equipment for TEM and SEM sample preparation. The Centre of Excellence NAMASTE contributed to the equipment for electron microscope with a CCD camera and an ADF (annular dark field) detector for the JEM-2010F microscope and an EBSD system for the JSM-7600F. Additionally, the IJS is a co-owner of a JEM-ARM200F (transmission electron microscope with atomic resolution) at the National Institute of Chemistry. Furthermore, the CEMM helps with the maintenance of the dual-beam SEM/FIB (focused ion beam) microscope (Helios Nanolab 650) at the Nanocenter department.



Prof. Miran Čeh

The research involving the staff and equipment at the CEMM is diverse regarding the investigated materials and the methods used. Scanning electron microscopy is employed to observe the morphology and structure of the surfaces and for the microstructural investigation and determination of the chemical composition. The most

frequently investigated samples are ceramics (polycrystalline oxide and non-oxide compositions), nanostructured materials, 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 wavelength dispersion (WDXS) spectrometer for X-rays, allowing a nondestructive determination of the chemical composition of the investigated materials. The scanning electron microscope JSM-7600F is additionally equipped with an electron back-scatter 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 (atomic level). Transmission electron microscopy enables structural and chemical analyses of the grain boundaries and the study of precipitates, planar defects and dislocation determinations. Instead of ceramic samples, also different material and structures are investigated like thin films on different substrates, alloys, delicate metallic magnetic materials, polymers, etc. 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 scanning transmission electron (STEM) unit, EDXS and EELS (electron energy loss) spectrometers, and a CCD camera. The CEMM also manages the necessary equipment for SEM and TEM sample preparation.

The operation of the centre is managed by properly trained employees. Besides maintenance of the equipment, among the other CEMM activities are trainings for new operators, organization of workshops and conferCEMM workshops for new operators: the aim of the workshops is to present the operation and handling with the equipment and to present properly prepared samples.



Figure 1: 7th CEMM Workshop (Koblar M, CEMM)

ences 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 IJS, as well through publications in traditional and digital media. For users of the microscopes the CEMM organized the 6th and 7th workshop (SEM sample preparation and scanning electron microscopy with microanalysis - EDS and WDS). The aim of the workshops is to present the operation and handling of the equipment, as well as presenting properly prepared SEM samples (Figure 1).

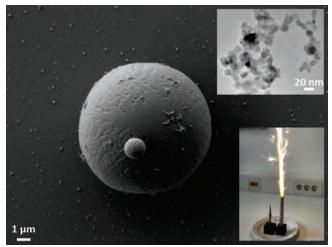


Figure 2: Fontana's experiment. (Koblar M, CEMM)

### In a collaboration with the projects ISO-FOOD and SmartNanoTox we have studied and analysed nanoparticles that are harmful for health.

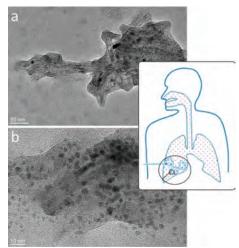


Figure 3: TEM analysis of proteins from the LA-4 cell layers. (a) Typical aggregate of LA-4 cell membrane and (b) nanoparticles after 2 days of incubation (Drev S, CEMM)

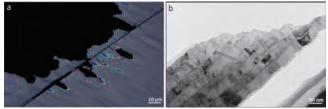


Figure 4: Study of the preferential sputtering effects in the depth profiling of multilayers. (Drev S, CEMM)

### **ISO-FOOD Spring School**

The ISO-FOOD Spring School and Workshop was devoted to various perspectives of nanoparticles in food that may appear during production, packaging or cooking. They can be added inadvertently or deliberately to improve the taste, colour, etc. Due to their size they are difficult to detect with simple experiments in the laboratory, so the electron microscopes were used. The size evaluation and chemical identification were defined using SEM, TEM and EDXS. Figure 2 shows today's popular fountains that are used at birthday parties. Particles that are produced can either pass into the respiratory system and a part of them can be transferred to the food, e.g., cake. We have shown that the particles are in different ranges of magnitude, from a few nanometres (TEM image) to micrometres (SEM image).

#### SmartNanoTox

The SmartNanoTox project explores the interactions between nanomaterials and cells (the identification of molecular initiating events). The production of new materials, in the world of science, is growing and their impact on health is often unexplored. The project includes the research of nanoparticles' inhalation and cardiovascular disease. A major part of the research is the explanation of molecular mechanisms. The CEMM has collaborated with TiO<sub>2</sub> nanoparticles' analysis using the transmission electron microscope JEM-2100. We have been focused on initiating the characteristics and typical morphology of the host material. With the F-5

department (Department of Solid State Physics) a few TEM samples of LA-4 epithelial cell layers were prepared and analysed. The TEM study indicated a typical aggregate of LA-4 cell membrane and nanoparticles after 2 days incubation of the LA-4 cell layer with nanoparticles in a complete cell-culturing medium. The nanoparticles, lipids and proteins can be identified with crystalline tube structures, the surrounding amorphous layer and the almost-round dark objects. (Figure 3)

The results and discussion of electron microscopy and other new technology combinations were published in the renowned journal (Urbancic. I.; Garvas. M.; Kokot. B.; Majaron. H; Umek. P; Cassidy. H.; Škarabot. M.; Schneider, F.; Galiani, S.; Arsov. Z.; Koklic. T.; Matallanas. D.; Čeh. M.; Muševič. I.; Eggeling. C.; Štrancar. J. Nanoparticles Can Wrap Epithelial Cell Membranes and Relocate Them Across the Epithelial Cell Layer. Nano Lett. 2018, 18, 5294-5305).

### Individual research work and analysis using the CEMM's equipment

Multilayer of Ag and Ni sputtered on a Si substrate. A TEM sample with the cross-section technique was prepared to analyse the preferential sputtering effect in the depth profiling of multilayers. A transmission electron microscope JEM-2010F was used to detected eight layers of Ag and Ni. A multilayer profile showed the constant thickness of particular layers. According to the AES (Auger electron spectroscopy) of a (Ag/Ni)x4/Si multilayer structure, the thicknesses of the layers are similar. The results of the AES and TEM techniques confirmed the thickness

of the layers (20-25nm). (Hofmann. S.; Zhou. G.; Kovač. J.; Drev. S.; Lian. S. Y.; Lin. B.; Liu. Y.; Wang. J. Y. Preferential sputtering effects in depth profiling of multilayers with SIMS, XPS and AES. Applied Surface Science (in press). (Figure 4)

A solid solution of  $Pb(Mg_{1/3}Nb_{2/3})O_3$ -xPbTiO<sub>3</sub> is a perovskite relaxor ferroelectric system with large polarization and strain responses to external fields. These are assigned to its special polar nanoscale distortions, which influence the movement of microscale ferroelectric domains. The transmission electron microscope JEM-2100 was used to detect a characteristic 90° tetragonal domain structure. Within the 90° domains, 180° domains (magnification: characteristic zig-zag pattern) and polar nanoregions are

embedded. (Otonicar. M.; Ursic. H.; Dragomir. M.; Bradesko. A.; Esteves. G., Jones. J. L.; Bencan. A.; Malic. B.; Rojac. T. Multiscale field-induced structure of (1-x)Pb(Mg1/3Nd2/3)O3-xPbTiO3 ceramics from combined techniques. Acta materialia. 2018, 154, 14-24). (Figure 5)

Scanning electron microscopy (JSM-7600F) was used to analyse the twin relation in SnO<sub>2</sub> ceramics. An EBSD map produced by the crystallographic orientation data from 3231 Kikuchi patterns recorded within the outlined

area. Selected grains are indicated by numbers and their angular relations are listed below. White lines indicate boundaries where the grains are met in the {101} twin orientation. Also, the MacKenzie plot of relative frequency of incidences among the SnO<sub>2</sub> grains has been made. The red lines indicate the incidence corresponding to the complementary angle of {101} twins in SnO<sub>2</sub>. (Tominc. S.; Rečnik. A.; Samardžija. Z.; Dražić. G.; Podlogar. M.; Bernik. S.; Daneu. N. Twinning and charge compensation in Nb<sub>2</sub>O<sub>5</sub>-doped SnO<sub>2</sub>-COO ceramics exhibiting promising varistor characteristics. Ceramics International. 2018, 44, 1603-1613). (Figure 6)

Superparamagnetic nanoparticles are currently under intensive investigation, being used for a variety of biological applications (bio separations), *in-vitro* cell manipulation, and magnetically targeted drug delivery.

(Kralj. S. and Makovec. D. The chemically directed assembly of nanoparticle clusters from superparamagnetic iron-oxide nanoparticles. Royal Society of Chemistry. 2014, 4, 13167-13171). Chains of superparamagnetic nanoparticles are coated with a silica layer containing large, radially oriented pores. The study of the superparamagnetic samples was made with the transmission electron microscope JEM-2100. (Figure 7)

## INTERNATIONAL PROJECTS

- H2020 EUROfusion Education-ED-FU Prof. Miran Čeh European Commission
- Micro-to Nanoscale Textures of Ore Minerals: Methods of Study and Significance Dr. Janez Zavašnik Slovenian Research Agency

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

- 1. Plasma-assisted wound treatment and topical introduction of molecules Dr. Janez Zavašnik
- Nanoscale investigations of diffusion controlled topotaxial phase transformations in rutile-corundum host systems Dr. Sandra Drey
- Advanced hydrodesulphurisation with catalyst nanomaterials Dr. Janez Zavašnik

## STAFF

Researcher

- 1. Prof. Miran Čeh, Head
- Postdoctoral associates
- 2. Dr. Sandra Drev
- 3. Dr. Jitka Hreščak
- 4. Dr. Janez Zavašnik, 17.09.18, transferred to Department K7 Postgraduates
- 5. Goran Miličić, B. Sc., left 17.03.18

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- 2. Mariola Brycht, Andrzej Leniar, Janez Zavašnik, Agnieszka Nosal-Wiercińska, Krzysztof Wasiński, Paulina Półrolniczak, Sławomira Skrzypek, Kurt Kalcher, "Synthesis and characterization of the thermally reduced graphene oxide in argon atmosphere, and its

application to construct graphene paste electrode as a naptalam electrochemical sensor", *Analytica chimica acta*, 2018, **1035**, 22-31.

- 3. Janvit Teržan, Petar Djinović, Janez Zavašnik, Iztok Arčon, Gregor Žerjav, Matjaž Spreitzer, Albin Pintar, "Alkali and earth alkali modified CuO<sub>x</sub>/SiO<sub>2</sub> catalysts for propylene partial oxidation: what determines the selectivity?", *Applied catalysis. B, Environmental*, **237**, 214-227.
- Petra Jenuš, Aljaž Iveković, Matej Kocen, Andreja Šestan, Saša Novak, "W<sub>2</sub>C-reinforced tungsten prepared using different precursors", *Ceramics international*, 45, 6, 7995-7999.
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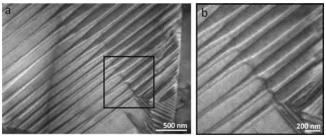
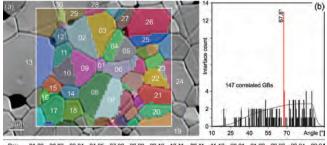


Figure 5: Domain structure of  $Pb(Mg_{1/3}Nb_{2/3})O_3$ -xPbTi $O_3$  sample (Otoničar M, K5)



 Pair
 01-02
 02-03
 03-04
 04-05
 07-08
 06-09
 09-10
 10-11
 11-12
 20-21
 21-22
 22-23
 23-24
 22-24

 Angle
 80.2
 67.8
 85.9
 67.7
 67.7
 72.6
 67.8
 68.3
 44.2
 33.1
 33.9
 68.0
 67.9
 68.3
 90.0

 Figure 6: Twin relation analysis in SnO, ceramics (Samardžija Z, K7)
 80.0
 67.9
 68.3
 90.0
 70.0
 70.0

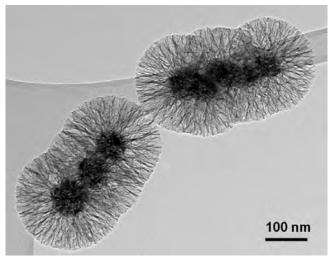


Figure 7: Superparamagnetic nanoparticles (Kralj S, K8)

 Andreja Šestan Zavašnik, B. Sc. Technical officer
 Maja Koblar, B. Sc. bearing calcite in a shallow, calcareous lake", *Earth and planetary science letters*, 2018, **496**, 20-28.

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- Rathish Rajan, Egidija Rainosalo, Selvin P. Thomas Thomas, Sunil Kumar Ramamoorthy, Janez Zavašnik, Jyrki Vuorinen, Mikael Skrifvars, "Modification of epoxy resin by silane-coupling agent to improve tensile properties of viscose fabric composites", *Polymer bulletin*, 2018, **75**, 1, 167-195.

# 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. The Centre has thirteen researchers and technical staff working in the areas of research results dissemination and eLearning. In particular, the centre is well known through the portals: VideoLectures.NET with multimedia materials of numerous scientific events, on-line training materials, and collection of tutorials on different scientific fields; ScienceAtlas.ijs.si and IST-World.Org for the analysis and visualization of large bibliographic and project databases. The Centre is covering the management, training and dissemination activities of several EU projects.



In 2018 we were active in the following projects from the H2020 program: EDSA (European Data Science Academ), OPTIMUM (Multi-source Big Data Fusion Driven Proactivity for Intelligent Mobility), MOVING (TraininG towards a society of data-saVvy inforMation prOfessionals to enable open leadership Innovation), EW-SHOPP (Supporting Event and Weather-based Data Analytics and Marketing along the Shopper Journey), EUBUSINESSGRAPH Mitja Jermol, M. Sc. (Enabling the European Business Graph for Innovative Data Products and Services), PRESTOCLOUD (Proactive Cloud Resources Management at the Edge for Efficient Real-Time Big Data Processing), WATER4CITIES (Holistic Surface Water and Groundwater Management for Sustainable Cities), MEET CINCH (A Modular European Education and Training Concept In Nuclear and RadioCHemistry), X5GONE (Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network), THEYBUYFORYOU (Enabling procurement data value chains for economic development, demand management, competitive markets and vendor intelligence), DATABENCH (Evidence Based Big Data Benchmarking to Improve Business Performance), PerceptiveSentinel (BIG DATA Knowledge

Extraction and re-creation Platform), ELEXIS (European Lexicographic Infrastructure), SILKNOW (Silk heritage in the Knowledge Society: from punched cards to big data, deep learning and visual/zangible simulations), COG-LO; (COGnitive Logistics Operations trough secure, dynamic and ad-

#### In 2018 the Centre for knowledge transfer in IT was actively involved in 18 European projects.

hoc collaborative networks), EnviroLENS; Copernicus for envir law enforcement support ) and ERASMUS+: Micro HE (Support Future Learning Excellence through Micro-Credentialing in Higher Education) and MentorTrain (Training and Equipping Mentors in SMEs to provide Quality Apprenticeships)

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, and marketing. 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 the 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:// videolectures.net/. It now offers 25,431 recorded tutorials from different scientific events. The main purpose of the portal is to provide free and open access to high-quality video lectures presented by distinguished scholars and scientists at the most important and prominent events. In today's world VideoLectures.NET represents a free knowledge hub, a way of opening up education to everyone for everyone and as there is a great need to share educational content on all levels in order to benefit society and foster the economy. It also provides a learning opportunity to audiences at all social levels.

VideoLectures.Net has strong connections to the Open Cast Foundation, Open Course Ware Consortium and Knowledge 4 All Foundation Ltd.

Videolectures.Net recorded and published 1664 new individual lectures in 2018. The majority of this content was produced by us, while 20 smaller-scale events were produced externally and submitted to us for publishing. The biggest events that we recorded and published in 2018 were:

Conference KDD2018 (544 lectures), ISWC2018 Conference (83 lectures), Summer school DLSS2018 (30 lectures), ESWC2018 Conference (88 lectures). In addition, a substantial amount of content was published based on long-term cooperations established with institutions such as NiB, Chemistry Institute of Slovenia, the CLARIN ERIC organization, University of Nova Gorica, Faculty of Architecture at the University of Ljubljana, EnetConnect Cost action and smaller events we continuously record at the JSI and in cooperation with other organizations in Slovenia and abroad.

Our Center is collaborating with the Department of Environmental Sciences at the JSI in the development and design of extensive courses in the field of radiochemistry. For that purpose we have recorded and published 34 courses in the scope of the project "A Modular European Education and Training Concept In Nuclear and Radio-CHemistry Courses" (Meet-Cinch).

In March 2018 we organized the 13th Student Competition in Computer Science, attended by 230 students from Slovenian secondary schools. We also organized project meetings for the EU project Elexis, a workshop ELRC "European Language Resource Coordination" and coorganized the "Open education designed" workshop, held in Vipava in Slovenia.

UNESCO Chair on Open Technologies for OER and Open Learning (Chair) and University of Nova Gorica started managing a free international online "Open Education for a Better World" mentoring programme. The first round took place from January to July 2018. The goal of the program is to design and implement OERs that will unlock potentials and bring benefits to many at no cost to the participants.

In the first round forty mentors applied to guide the candidates in preparing their online courses. Mentors come from all around the world.

Fourteen developers with concrete ideas for open educational resources (OER) aligned with Sustainable Development Goals (SDGs) were chosen to be guided on-line towards the implementation of their OER. Applications



Figure 1: Participants of the Open Education Design course in Vipava, July 2018

come from all over the world, namely Brazil, Canada, Fiji, India, Italy, Kenya, Liberia, Nigeria, Slovenia, South Africa, USA and Uzbekistan. The OERs are available in different languages.

Following success of the mentoring programme in 2017/2018 we published a 2018/2019 Call in autumn 2018. We received 40 applications as developers and 50 applications as mentors from all around the world. As a result of the increased number of projects to be supported in 2019 as well as different time zones, the organisers have decided to establish 3 OE4BW hubs, namely OE4BW Hub covering North and South America, OE4BW Hub covering Africa and Europe and OE4BW Hub covering Asia to coordinate projects from the region.

Together with the University of Nova Gorica our Unesco Chair organized a 5-day course on Open Education Design in Lanthieri Mansion in Vipava. The aim of the course was to equip the participants with basic knowledge, practical advice and hands-on experience to prepare them for their own design of Open Educational Resources (OER). The participants became familiar with open-education design processes, methods and tools.

They learned how to align open education with developmental and strategic goals. They got basic knowledge about open education concepts, about pedagogical and didactical issues as well as about content-related issues in open education. They learned from OER experts and practitioners. The course was attended by 50 participants from 17 countries, namely Slovenia, Brazil, Fiji, France, Greece, India, Italy, South Africa, Canada, Kenya, Macedonia, Malaysia, Malta, Germany, Uzbekistan, Great Britain and USA.

In 2018, we completed our fourth cycle of activities within the MyMachine project.

We completed work on two products and started new activities of developing prototypes. In June 2018 we organized an exhibition of the work we did in the academic year 2017/2018, with an outlook on planned activities. Our exhibition was held at RampaLab in Ljubljana, where we focused on conversations with students and pupils that are working on new prototypes.

The international collaborations concluded in the publication of a book, which is a collection of essays from world-renowned scholars and practitioners of project-based learning, creativity in education and open education to which MyMachine Slovenia contributed a chapter on open education.

In 2018, we acquired the data from the Business Register and public procurement data for the H2020 project TheyBuyForYou. We developed some methods for comparing documents (contracts) across different languages and started developing an application for the analysis of public procurement data.

In March, we started organizing lectures about information security. In 2018 we had 8 lectures under the title Infosec seminary. The main topic of the lectures is focused on information security, but the lectures were covering diverse themes. We had a lecture about the malware analysis with reverse engineering, a lecture about ensuring the integrity of data in digital forensics, we looked into modern encryption algorithms (X3DH and Double Ratchet),

listened to a lecture on cybercriminal, organized two lectures on security of cryptocurrencies, a lecture on cyberpower capabilities of North Korea and a lecture on the use of intrusive methods in the intelligence and investigation process. Two of the lecturers were also invited from the USA. The contents of the lectures are available on the web site https://infosec-seminar.si/, and the recordings of the lectures are also published on the Videolectures.net portal.

In 2018, we continued to work with Codeweek, the aim of which is to promote programming among youngsters. In January we participated in the Hokus pokus festival in Pionirski dom (in cooperation with Codeweek),

where we showed children the use of computers and sensors in chemical experiments and how computers can be used in traffic (we developed a simple traffic counter and speed measurement radar). A slightly expanded workshop for children on the same topic was repeated in October at the opening of Codeweek's month of programming. We also presented the use of sensors in chemistry to children who participated in the School of Experimental Chemistry, which has been organised in cooperation with the Slovenian Society of Chemistry Fans and co-workers from section K1 (Department of Inorganic Chemistry and Technology). Together with

Within the UNESCO Chair (http://unesco.ijs. si/), in cooperation with the University of Nova Gorica, we have successfully organized a free international summer online mentoring program titled "Elimination of Education for a Better World" (OE4BW), linking them to the United Nations' Sustainable Development Goals.

children we developed a simple pH meter, temperature sensor, particulate matter detector and a detector of various gases (including a simple alkotest), using a micro controller Arduino and various sensors. Children then carried out a series of chemical experiments with those sensors.

At the end of 2018, we signed a cooperation agreement with the Association of Electronics of Slovenia, in the field of development of education programs and mentoring of children about electronics and its use, and the development and testing of prototypes of electronic circuits. The Association of Electronics of Slovenia will be also publishing their educational lectures on the Videolectures.net portal.

In the same year we started with two mentorships within project SKOZ (Center for Career Orientation - West). This project is intended for gifted students from the western Slovenian region who, under the mentorship of researchers, are conducting their own research. Our department is involved in the mentoring of two groups of students.

The first group of students (where co-mentorship is conducted with a colleague from section K1), started the development of a detector of harmful gases in agriculture. Within the project, we developed a device that contains various gas sensors to detect the presence of harmful gases that occur in agriculture (e.g., carbon monoxide, carbon dioxide, methane, ammonia, various volatile organic compounds (VOCs), etc.). The device, for which we also developed an enclosure that was printed with a 3D printer, records the measurements to a database, and also sends the data to the end users via the web application.

Another group of students is developing a device for measuring temperature, humidity and UV index, which will inform users and issue a warning about the level of UV radiation in the environment via a built-in screen or Bluetooth. We developed both devices in cooperation with the Association of Electronics of Slovenia. We also introduced the process of designing a prototype electronic device and making a printed circuit board to students working on a project.

We continued with the Water4Cities project Integrated surface and groundwater management for sustainable urban development, which is a project within the framework of the European RISE project Horizon 2020 Marie Skłodowska Curie. We continued to collect and analyse data on the example of Ljubljana and the Greek island of Skiathos, with the help of which we are developing models and a platform that will enable the monitoring of urban water resources in real time. This will contribute to optimal water management and minimize environmental and ecosystem impacts. In 2018, we attended and recorded a special session dedicated to the Water4Cities project, which took place during the EWAS conference in Lefkada, Greece. We also record video and edit regular webinars and interviews with researchers involved in the project. All the recordings are hosted on the Videolectures.NET portal.

The H2020 project MOVING (TraininG towards a society of data-saVvy inforMation professionals to enable open leadership INnovation) is in its final year. CT3 with the involvement of E3, was mostly active in producing video demonstrations about the developed technologies, services and the MOVING platform, for the purpose of dissemination and exploitation activities. The videos also serve for the didactic and curricula development in the MOVING platform, that enables its users to improve their information literacy by training how to exploit data-mining methods in their daily research tasks. Its novel integrated working and training environment supports the education of data-savvy information professionals and allows them to address the big-data and open-innovation challenges. Moreover, the MOVING consortium has been working on developing new and more effective methods for lecture video fragmentation and fragment-level annotation, to allow for fine-grained access to lecture video collections. In the latest MOVING method, developed by partner CERTH, automatically generated speech transcripts of the lecture video are analysed with the help of word embeddings that are generated from pre-trained state-of-the-art neural networks. This lecture video fragmentation method is part of the MOVING platform, and its results are also being

included in the VideoLectures.NET portal, making it possible for the users of both platforms to access and view specific fragments of lecture videos that cater to their information needs.

We became partners in the Erasmus + project "Training and Equipping Mentors in SMEs to provide Quality Apprenticeships" (Mentortrain), in which we will participate with the online repository Videolectures.net. At the beginning of the project, the first consortium meeting defined the cooperation between the partners and the implementation of tasks, namely recording educational content in the field of apprenticeships and mentoring in companies.

Work on project "Support Future Learning Excellence through Micro-Credentialling in Higher Education" (MicroHE) focused in 2018 mostly on tasks of the technical work package, which we are leading. In 2018 we achieved two distinctive and complementary objectives. The first was the creation of the micro-credentials metadata standard and the initial design of building a micro-credentials clearinghouse. The main output in 2018 was, therefore, a Draft of a metadata standard to record ECTS/learning modules and the facilitation of the required public consultation.

### Organization of conferences, congresses and meetings

- 1. Project meeting of the EU project ELEXIS, 15.-17.2. 2018
- 2. 13th Student competition in computer science, Ljubljana, Ljubljana, 24. 3. 2018
- 3. Organization of the workshop ELRC, Ljubljana, 24. 4. 2018
- 4. Co-organization of the workshop "Open education Design" Vipava, 2.-6.7. 2018

## INTERNATIONAL PROJECTS

- 1. ERASMUS+: Micro HE Support Future Learning Excellence through Micro-Credentialing in Higher Education
- Mihajela Črnko
- European Commission ERASMUS+: MentorTrain - Train
- ERAŠMUS+; MentorTrain Training and Equipping Mentors in SMEs to provide Quality Apprenticeships Mihajela Črnko
- European Commission
- 3. H2020 EDSA; European Data Science Academy
- Mitja Jermol, M. Sc. European Commission
- H2020 OPTIMUM; Multi-source Big Data Fusion Driven Proactivity for Intelligent Mobility
  - Dr. Matej Kovačič
  - European Commission
- H2020 MOVING; Training Towards a Society of Data-Savvy Information Professionals to enable Open Leadership Innovation Dr. Tanja Zdolšek Draksler
  - European Commission
- H2020 STEM4youth; Promotion of STEM Education by Key Scientific Challenges and their Impact on Our Life and Career Perspectives
- Dr. Matej Kovačič
- European Commission
- 7. H2020 PrEstoCloud; Proactiive Cloud Resources Management at the Edge for Efficient Real-Time
  - Mitja Jermol, M. Sc.
  - European Commission
- H2020 euBusinessGraph; Enabling the European Business Graph for Innovative Data Products and Services
   Mitig Jarmad M. Sc.
  - Mitja Jermol, M. Sc. European Commission
- H2020 EW-Shopp; Supporting Event and Weather-based Data Analytics and Marketing along the Shopper Journey
- Mitja Jermol, M. Sc.
- European Commission
- H2020 Water4Cities; Holistic Surface Water and Groundwater Management for Sustainable Cities Mitja Jermol, M. Sc.
- European Commission
- 11. H2020 MEET-CINCH; A Modular European Education and Training Concept in Nuclear and RadioChemistry
- Mihajela Črnko European Commission
- H2020 X5gon; Cross Modal, Cross Cultural, Cross Lingual, Cross Domain, and Cross Site Global OER Network Mitia Jermol. M. Sc.
  - European Commission

- 13. H2020 PerceptiveSentinel; BIG DATA Knowledge Extraction and Re-creation Platform Mitja Jermol, M. Sc.
- European Commission 14. H2020 - DataBench; Evidence Based Big Data Benchmarking to Improve Business Performance
  - Mitja Jermol, M. Sc.
  - European Commission
- H2020 TheyBuyForYou; Enabling Procurement Data Value Chains for Economic Development, Demand Management, Competitive Markets and Vendor Intelligence Dr. Matej Kovačič European Commission
- H2020 SILKNOW; Silk Heritage in the Knowledge Society; From Punched Cards to Big Data, Deep Learning and Visual/Tangible Simulations Mitja Jermol, M. Sc.
  - European Commission
- 17. H2020 COG-LO; COGnitive Logistics Operations through secure dynamic and ad-hoc collaborative networks
  - Mitja Jermol, M. Sc.
  - European Commission
- H2020 EnviroLENS; Coprenicus for Environmental Law Enforcement Support Mitja Jermol, M. Sc. European Commission
- H2020 ELEXIS; European Lexicographic Infrastructure Mitja Jermol, M. Sc. European Commission

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

- 1. Videorecording and Post-Processing Mitia Jermol, M. Sc.
- CLARIN European Research Infrastructure for Language Resources and Technology Mitja Jermol, M. Sc.
- Clarin Eric 3. European Language Resource Coordination (ELRC) Workshop 2018, JSI, Ljubljana, Slovenia, 24,4,2018
- Mitja Jermol, M. Sc. Dfki Gmbh - Deutsches Forschungszentrum fuer
- Recording, Publishing and Disseminating of the Scientific Content of the EnetCollect Project on Videolectures.net Mihajela Črnko
- Eurac Research
- US-Slovenia S&T Cooperation Overview Dr. Matej Kovačič
- Embassy of the United States of America

## **STAFF**

- Postgraduate 1. Anja Polajnar, B. Sc. Technical officers
- Mitja Jermol, M. Sc., Head
   Dr. Matej Kovačič
   Dr. Ervin Pfeifer\*
   Matjaž Rihtar, B. Sc.
   Dr. Tanja Zdolšek Draksler

# **BIBLIOGRAPHY**

### **ORIGINAL ARTICLE**

1. Tanja Zdolšek, Karin Širec, "Conceptual research model for studying students' entrepreneurial competencies", *Naše gospodarstvo: revija za aktualna gospodarska vprašanja*, 2018, **64**, 4, 23-33.

#### Technical and administrative staff

- Aleš Buh
   Mihajela Črnko

- Mihajela Cruko
   Ana Fabjan, B. Sc.
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   Davor Orlić, B. Sc.
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   Špela Sitar, B. Sc.

# MILAN ČOPIČ NUCLEAR TRAINING CENTRE ICJT

The mission of the ICJT training centre is training in the field of nuclear technologies and radiation protection. In addition, the ICJT is actively informing the public about those technologies.

Training in the area of nuclear technologies is our primary mission. Two courses *Basics of Nuclear technology* (OTJE) were held. This course is intended for general technical staff of Krško NPP, as well as for technical support organizations, regulatory bodies, etc. There was no longer a course on *Nuclear technology* (TJE), which is the initial training of future control-room operators. There were also two courses *Nuclear Energy in Short* (JEK), intended for administrative and financial staff of the NPP. For the Qtechna company we have conducted a one-week course Nuclear technology fundamentals (OJT).

There were 25 radiological protection training courses for the medical, industrial and research use of radioactive sources.

In collaboration with the Reactor physics division and the Reactor infrastructure center, an **international course** was organized in the area of the safety of research reactors.

Public information remains an important part of our activities. Groups of visitors (mainly school children, Head: students and various societies) were regularly attending lectures and visiting the permanent exhibition on nuclear **Dr. Igor Jenčič** 

energy; smaller groups also visited the TRIGA reactor and/or the accelerator. The lectures were offered on electricity from nuclear energy, fusion, isotopes, energy in general, and a new lecture on the use of radiation in industry, medicine and research. Altogether, there were 162 groups or 6499 visitors this year. Since 1993, a total of 181,379 pupils, teachers and others, visited our information centre. We have continued monitoring and analysing media reports on nuclear energy.





Figure 1: Summer workshop about energy for a group of young visitors



Figure 2: President of the American Nuclear Society (ANS), Dr. John Kelly, lecturing about the American response to the Fukushima accident



Figure 3: Opening of The Basic Nuclear Technology Course



Figure 4: Training of future nuclear professionals includes a demonstration of the NPP Krško simulator



## Table of training activities at the Nuclear Training Centre in 2018

Date	Title of the course	Partici- pants	Lecturers	Weeks	Participants × weeks
5.02 7.02.	Radiation protection for baggage-screening systems	7	2	0.4	2.8
5.03 7.03.	Radiation protection for industrial and other practices (measurement of road- way density and humidity)	2	4	0.6	1.2
5.03 7.03.	Radiation protection for High-Activity Sealed Sources	1	4	0.6	0.6
5.03 7.03.	Radiation protection for handheld XRF spectroscopy	6	4	0.6	3.6
5.03 9.03.	Radiation protection for industrial and other practices (radiography)	12	4	1	12
12.03.	Radiation protection for baggage-screening systems	4	4	0.2	0.8
12.03.	Radiation protection for industrial and other practices	8	4	0.2	1.6
12.03 13.03.	Radiation protection for industrial and other practices (unsealed sources)	7	5	0.4	2.8
12.03 14.03.	Radiation protection for medical and veterinary workers - Nuclear medicine workers	6	5	0.6	3.6
15.03.	Radiation protection for baggage-screening systems - Refresher Course	4	4	0.2	0.8
15.03.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	1	5	0.2	0.2
15.03.	Radiation protection for industrial and other practices - Refresher Course	8	4	0.2	1.6
15.03.	Radiation protection for handheld XRF spectroscopy - Refresher Course	1	4	0.2	0.2
15.03.	Radiation protection for industrial and other practices (measurement of road- way density and humidity) - Refresher Course	4	4	0.2	0.8
15.03 16.03.	Radiation protection for industrial and other practices (radiography) - Re- fresher Course	3	4	0.2	0.6
7.05 5.06.	Basics of nuclear technology, theory	25	11	4.2	105
6.06 29.06.	Basics of nuclear technology, systems	26	7	3.6	93.6
13.06 14.06.	Nuclear Energy in Short	5	4	0.4	2
26.09 27.09.	Nuclear Energy in Short	15	4	0.4	6
1.10 5.10.	Training Course on "Requirements and safety evaluation of Research Reactors"	13	10	0.8	10.4
1.10 30.10.	Basics of nuclear technology, theory	7	13	4.2	29.4
8.10 10.10.	Radiation protection for High-Activity Sealed Sources	1	4	0.6	0.6
8.10 10.10.	Radiation protection for handheld XRF spectroscopy	5	4	0.6	3
8.10 12.10.	Radiation protection for industrial and other practices (radiography)	1	4	1	1
15.10.	Radiation protection for industrial and other practices	7	3	0.2	1.4
15.10 16.10.	Radiation protection for industrial and other practices (unsealed sources)	2	4	0.4	0.8
15.10 18.10.	Radiation protection for medical and veterinary workers - Nuclear medicine workers	3	6	0.6	1.8
18.10.	Radiation protection for industrial and other practices (unsealed sources) - Refresher Course	6	5	0.2	1.2
18.10.	Radiation protection for industrial and other practices - Refresher Course	7	4	0.2	1.4
18.10.	Radiation protection for handheld XRF spectroscopy - Refresher Course	1	4	0.2	0.2
18.10.	Radiation protection for industrial and other practices (measurement of road- way density and humidity) - Refresher Course	1	4	0.2	0.2
22.10 26.10.	Nuclear technology fundamentals	9	4	1	9
5.11 28.11.	Basics of nuclear technology, systems	10	7	3.4	34
TOTAL		218	163	28	334.2

## INTERNATIONAL PROJECT

- 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
- Strengthening the Competence of Entrepreneurship and Promoting Flexible Transition between Education and the Environment in Primary and lower Secondary Schools Tomaž Skobe, M. Sc.
- Ministry of Education, Science and Sport
  Strengthening the Competence of Entrepreneurship and Promoting Flexible Transition between Education and the Environment in Secondary Schools Tomaž Skobe, M. Sc.
- Ministry of Education, Science and Sport
  ENRAS: Ensuring Radiation S afety for First Responder Teams in Case of Radiological or Nuclear Accidents Matjaž Koželj, M. Sc.

Government Office for Development and European Cohesion Policy

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

1. Trainings of the RZ for Foreign Market Matejka Južnik, M. Sc.

## STAFF

#### Researcher

- 1. Dr. Igor Jenčič, Head
- Technical officers
- 2. Jure Hribar, B. Sc., left 07.05.18
- 3. Matjaž Koželj, M. Sc.
- 4. Tomaž Skobe, M. Sc.

- Training of MIT Dedicated Practical Educational Course "Experimental reactor physics", Jožef Stefan Institute, Ljubljana, Slovenia, 26 March to 30 March 2018 Dr. Igor Jenčič Massachusetts Institute of Technology (MIT)
- Training Courses TJE and OTJE For Foreign Participants Dr. Igor Jenčič

## NEW CONTRACTS

- 1. Small services in year 2018
- Matejka Južnik, M. Sc. 2. Operation of the Nuclear Information Centre in 2018
- Dr. Igor Jenčič Gen energija, d.o.o.
- Basic Training Course on Nuclear Technology and Nuclear Power Plants Dr. Igor Jenčić
- ICJT Training Programme implementation in the year 2018 Dr. Igor Jenčič
- Nuklearna Elektrarna Krško d. o. o.
- 5. Trainings of the Radiation protection Matejka Južnik, M. Sc.
- 5. Vesna Slapar Borišek, B. Sc.
- 6. Luka Tavčar, B. Sc., 01.07.18, transferred to Department CEU
- Technical and administrative staff
- 7. Saša Bobič
- 8. Matejka Južnik, M. Sc.
- 9. Borut Mavec, B. Sc.

# 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 work in the reactor with the Hot Cell Facility and we are authorised by the regulatory authority to perform environmental monitoring.

SVPIS also controls 17 laboratories that use sources of ionising radiation in their research work. There are different sources of radiation used, such as sealed sources, open sources, X-ray units and the accelerator TANDETRON, which need regulatory control. Furthermore, we are involved in radioactive waste management.

SVPIS is authorized by the Slovenian radiation protection administration and nuclear safety administration to perform control in industrial and research institutions dealing with open or sealed radioactive sources and X-ray units.

The measurements of dose rate, contamination and gamma spectrometry are performed usingan accredited method (LP-022, EN ISO/IEC 17025).Maty



Matjaž Stepišnik, M. Sc.

#### Personal dosimetry

Personal doses of 118 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters. The maximum individual yearly dose was 0.41 mSv. This is only 2 % of the regulatory limit for occupational exposure (20 mSv per year) and 41 % of the limit for the public (1 mSv per year). The collective dose at the JSI in 2018 was 3.6 man-mSv.

#### Supervision of the 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. Locally elevated radiation levels could be measured mostly in the reactor controlled area.

At present, 100 sources of radiation are in use, which require regulatory control and additionally there are 438 low-activity sources in different laboratories.

In 2018, 19 radiological 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.

#### Environmental monitoring of the reactor

The environmental monitoring of the Reactor Center was performed according to the existing program. The program consists of effluent measurements and measurements of samples in the environment. The activity concentrations of gamma emitters in water samples, filters, noble gases, soil samples and sediment samples were measured periodically. About 370 different samples were measured with gamma spectrometry. Environmental passive dosimeters were 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 2018 due to activities at the Reactor Center was insignificant.

### Expert assessments and measurements for outside customers

The Radiation Protection Unit is authorized for supervision measurements and expert assessments in the field of radiation protection. In the past year several radiological control investigations were carried out in industrial and research institutions. Our group has participated in the evaluation of the radiological monitoring of Krško NPP, the Research Reactor TRIGA and storage for low- and intermediate-level waste in Brinje.



## STAFF

Technical officers

- 1. Dr. Tinkara Bučar
- Eva Kalšek, B. Sc., left 15.05.18
   Matjaž Stepišnik, M. Sc., Head

### Technical and administrative staff

- 4. Thomas Breznik, B. Sc.
- Tanja Murn, B. Sc.
   Nina Udir, B. Sc.

# **BIBLIOGRAPHY**

## INDEPENDENT COMPONENT PART OR A CHAPTER IN A

### MONOGRAPH

1. Matjaž Stepišnik, "Radionuklidi v reki Savi", In: Benjamin Zorko (ed.), et al., Ugotavljanje radioaktivnosti v okolju v okolici NEK po zagonu HE Brežice, 2018, 1-19.

# CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION

Established in 1996, the Office of Technology Transfer was transformed in January 2011. Based on its work 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 industry, 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.

The Center's success is based on the work of 16 professionals, 7 of which are educated in natural sciences and engineering, 6 in economics, 3 in law and 1 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 three team members hold the U.S. "Certified Licensing Professional" certificate. The Head: head of the group has the titles of Latin Legum Magister (LLM), Master of Business Administration (MBA) and Dr. Špela Stres, MBA, LLM Registered Technology Transfer Professional (RTTP).

Our important tool is a created network of contacts 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. Our clients are primarily JSI researchers, although numerous companies and other research organisations have also been known to procure our services in 2018.

Marketing of 20 JSI technologies, procedures for the creation of two spin-out companies, 107 identified RR topics.

In 2018 the Center for Technology Transfer and Innovation was partly funded through five larger and numerous smaller EU and national projects. The projects belonged to various funding programmes and schemes: Enterprise Europe Network (EEN) Slovenia and EEN Scaleup (COSME scheme), EEN We4SMESLO and KET4Clean Production (Horizon 2020), Scale(up) Alps (INTERREG Alpine Space), SYNERGY and KETGATE (INTERREG Central Europe), Co-Create and finMED (INTERREG MED), and projects connected to science in the school system: NOCMOC, ICYDK and STEM4Youth (Horizon 2020). Project activities were connecting and completing our core TT activities.

In 2018, CTT faced several activity-related challenges, the largest of which were: (i) preparation, negotiation, and successful application for establishing a Consortium of Technology Transfer (KTT), covering all the largest Slovenian PROs, and led by CTT, and (ii) successful application to the call for Execution of support services by the innovation ecosystem actors in Slovenia in 2018 and 2019. At the 11th International Conference on Technology Transfer, there was a ceremony for awarding the best innovations.

Internally, CTT is divided into four groups, whose activities mutually interact with, and complement, each other.

Group for protection and marketing of intellectual property deals with cases that were applied through the single entry point (31 cases), gives first advice to researchers (26), prepares assessments of patentability - reviews state of the art (18). The number of these activities has risen considerably in comparison with the previous year. The group also evaluates

2000 visitors during the Open Day at the JSI, 68 school visits, 500 visitors during the Researchers' Night.



Figure 1: Jožef Stefan Institute Open Day, JSI, Ljubljana, Slovenia, 24. 3. 2018

market potential, helps prepare the invention for disclosure within the research organisation (18), helps draft the patent applications, prepares agreements on the ownership of intellectual property (9), advises on the choice of patent attorney, prepares and files the patent application and gives advice about the strategy of the international (7) and national (7) expansion of patent protection. The group also takes care of the active marketing of IJS technologies (20 technologies promoted to more than 300 enterprises and other organisations, 19 technologies promoted through the Enterprise Europe Network). It manages received interests (78) and starts the negotiations (15). It



Inducted by the JRC into the TTO Circle, the group of PROs most active in the field of knowledge and technology transfer (including the institutes Max Planck, Weitzman, Fraunhofer, VITO, VTT). Some of the best-rated commercialization experts of the European Commission.



Figure 2: Entrepreneurial education for young researchers 2018 spring, JSI, Ljubljana, Slovenia, 24. 5. 2018

Successful application to the call for Execution of support services by the innovation ecosystem actors in Slovenia in 2018 and 2019.

markets technologies through making expressions of interest towards other published profiles (78). Moreover, group members arrange for the signing of non-disclosure agreements (16), manage affairs with partners in different consortia (7), take part in negotiations (15), prepare license agreements (8) 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 2018 two spin-out companies were created.

The above-mentioned group closely cooperates with the **Group for contractual collaboration with industry**, which visits both large and small companies (43 in 2018), organises their return visits to the JSI (20), organises sector and regional visits of companies to JSI and collaborates with other support environment entities. This group's members are trying to find new topics for cooperation within the development projects among companies and researchers (107), prepare technology offers, arrange for the signing of non-disclosure agreements and acquire written consent for further international cooperation with business or technology-research goals (15). The group also takes part in various events; in the course of the 11th International Technology Transfer Conference it organised individual meetings between companies and researchers (40).

Group for promotion, education and project management has prepared and disseminated lists of Slovenian and EU tenders (12) and foreign partner searches, helped prepare project applications, especially in the "Exploitation" and "Dissemination" part, weekly disseminated other information to TT coordinators, which has efficiently contributed to the

application of new projects with foreign partners (4). The group has successfully spread various information through the CTT e-newsletter and CTT's Facebook profile, organised an Open Day at JSI (2000 visitors), within the European Researchers' Night attracted 500 visitors to demonstrations and interviews with scientists, organised 60 school visits at the JSI, provided two entrepreneurial education sessions for young researchers (39 participants in total), and organised the 11th International Technology Transfer Conference.

Organisation of the 11<sup>th</sup> International Technology Transfer Conference – more than 100 visitors, competition for the best innovation idea, international visit from Slovenia, EU countries, 40 B2R meetings.



Figure 3: 11<sup>th</sup> International technology transfer conference, JSI, Ljubljana, Slovenia, 8.–12. 10. 2018

Group for research in the field of technology transfer and innovation

We operate as valuators and external experts in the frame of the European Commission for different respectable international institutions (Academy of Science Finland; Federal Ministry of Science, Research and Economics, Austria; Investment Fund South East Europe, MGRT, ERC). We were recognized by the JRC as one of the most propulsive technology transfer offices in the EU and were included into the TTO Circle, the group of PROs most active in the field of knowledge and technology transfer (including the institutes Max Planck, Weitzman, Fraunhofer, VITO, VTT). As one of the best-rated commercialization external experts in EU we work for the European Commission and advise different consortia within H2020, with the emphasis on program Industrial Leadership (FoF, NMP, ICT). The HiPEAC Network of Excellence awarded the group head the Technology Transfer Award for the technology transfer project "A technology radiation dosage manipulation and surveillance".

## Organization of Conferences, Congresses and Meetings

 Meeting with Ms. Isabelle de Sutter, Systematic Paris Region Digital Ecosystem, JSI, Ljubljana, Slovenia, 23. 1. 2018

- "Co-Create" training for companies in the furniture and metal-tool industry, JSI, Ljubljana, Slovenia, 25.
   1. 2018
- 3. Study visit under the KETGATE project, JSI, Ljubljana, Slovenia, 31. 1. 2018
- 4. Jožef Stefan Institute Open Day, JSI, Ljubljana, Slovenia, 24. 3. 2018
- 5. Entrepreneurial education for young researchers 2018 spring, JSI, Ljubljana, Slovenia, 24. 5. 2018
- 6. Cross-fertilization event in the context of InterregMED Co-Create project, JSI, Ljubljana, Slovenia, 15. 6. 2018
- 7. "EU-GIVE" project 1. meeting of stakeholders in a collaborative economy in Slovenia, JSI, Ljubljana, Slovenia, 15. 6. 2018
- 8. Conference for researchers, small enterprises and actors of the co-operative economy (within the SYNERGY project), IJS, Ljubljana, Slovenia, 15. 6. 2018
- 9. "KETGATE" Workshop RTOs, JSI, Ljubljana, Slovenia, 4. 7. 2018
- 10. Sources of Finance for Scale-up and Start-up Companies & Collaborative Economy as a Form of Support for Companies (EU-GIVE Focus Group & Scale(up)Alps NITRO event), JSI, Ljubljana, Slovenia, 12. 9. 2018
- 11. Open-door evening at the Jožef Stefan Institute, JSI, Ljubljana, Slovenia, 28. 9. 2018
- 12. EEN Double Sector Group Meeting, JSI, Ljubljana, Slovenia, 8.-10. 10. 2018
- 13. 11th International technology transfer conference, JSI, Ljubljana, Slovenia, 8.-12. 10. 2018
- 14. Understanding the other side in the negotiation with industry, JSI, Ljubljana, Slovenia, 12. 10. 2018
- 15. Entrepreneurial education for young researchers 2018 autumn and Presentation the services of the Supportive Innovative Environment (SIO) to the researchers of the JRO, JSI, Ljubljana, Slovenia, 30. 11. 2018
- 16. Spin-out creation based on patents and innovation, JSI, Ljubljana, Slovenia, 7. 12. 2018
- 17. Raising awareness and promoting the process of commercialization of official inventions on PRO, JSI, Ljubljana, Slovenia, 12. 12. 2018
- 18. Connect with Jožef Stefan Institute and other technology centers Project KETGATE workshop for small and medium-sized enterprises, JSI, Ljubljana, Slovenia, 13. 12. 2018

# INTERNATIONAL PROJECTS

- K7, CTT ID Creations; Rights and Obligations regarding the Development, Use and Commercialization of Hydrothermally Synthetized TiO2 Coatings in Metal Orthopaedic and Dental Implants Dr. Scole Street
  - Dr. Špela Stres Id Creations Ov
- OPENISME; Open Platform for Innovative SMEs; EACI, CIP Programme Dr. Špela Stres
- European Commission
- COSME; EU-GIVE Generating Opportunities from Intangible Assets and Value Chains in the Collaborative Economy in Europe Dr. Špela Stres
- European Commission
- 4. COSME SGA2; EEN Slovenia 2; EEN Slovenia Services in Support of Business and Innovation in Slovenia
  - Dr. Špela Stres
  - European Commission
- COSME EEN Scaleup; EEN Slovenia in support to young Slovenian SMEs with high potential to scale-up Dr. Social Stress
  - Dr. Špela Stres European Commission
- 6. ICYDK In Case You Didn't Know
- Dr. Špela Stres EUIPO Intellectual Property Office
- H2020 STEM4youth; Promotion of STEM Education by Key Scientific Challenges and their Impact on Our Life and Career Perspectives Dr. Špela Stres
- European Commission
- H2020 KET4CleanProduction; Pan-European Access for man.SME on tech. services for clean production through a Network of premier KET Technology Centres with one stop shop access incl. EEN and discourse with policy makers on RI3 Dr. Spela Stres
  - European Commission
- 9. H2020 NOCMOC; European Researchers' Night (NIGHT) Dr. Špela Stres
- European Commission
- 10. H2020 We4SMESLO\_3; Enhancing the Innovation Management Capacity of SMEs (by EEN), Slovenia

Dr. Špela Stres European Commission

 H2020 - Umem4QC; Ultrafast Charge Density Wave Memory or Quantum Computing Dr. Špela Stres European Reasearch Council Executive Agency

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

- 1. Accelerate and promote the Alpine Space Start-up Ecosystem Dr. Špela Stres
- Interreg Alpine Space Programme 2. Co-Create: Setting up a network of COmpetitive MED Clusters with the contribution of cREATive Industries
- Dr. Špela Stres Interreg Med Programme
- Central European SME Gateway zo Key-enabling Technology Infrastructures Sparking new Transnational KET Innovation Ecosystem Dr. Špela Stres
- Interreg Central Europe Programme
- Synergic Networking for Innovativeness Enhancement of central european actoRs focused on hiGh-tech industry Dr. Špela Stres
- Interreg Central Europe Programme
- 5. Boosting the financing of innovation for green growth sectors through innovative clusters services in the MED area
- Dr. Špela Stres
- Interreg Med Programme
- The consortium for technology transfer from the PRO to the economy Dr. Spela Stres
   Nicitary of Planetics Optimized Science and Science
- Ministry of Education, Science and Sport
- Implementation od support activities for innovation ecosystem actors in Republic of Slovenia in the years 2018-2019 Dr. Špela Stres
- Ministry of Economic Development and Technology
- JSI Share of License Revenues related to Exploitation of Inventions Abroad (JSI License Revenue Share - Abroad) Dr. Špela Stres

## VISITORS FROM ABROAD

- Isabelle de Sutter, Responsible Europe Head of European Affairs Systematic Paris Region 1. digital Ecosystem, Paris, France, 23. 1. 2018
- 2. Majid Najafian, Representative of company ITEM Co, CEO of Iran Technology Export Mgmt.Co, Teheran, Iran, 14. 3. 2018
- Alan Mutka, Fakulteta za elektrotehniko in računalništvo, Bjelovar, Croatia, 21.-22. 3 3. 2018
- 4 Stjepan Golubić, Visoka tehnična šola - Oddelek za mehatroniko, Bjelovar, Croatia, 21.-22. 3. 2018

## STAFF

- Researcher 1. Dr. Špela Stres, MBA, LLM, Head
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- Technical officers
- Dr. Žiga Bolta, left 08.01.18 3.
- 4. Aleš Dragar, M. Sc., left 01.03.18
- Tomaž Justin, B. Sc. 5. Dr. Duško Odić
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- France Podobnik, B. Sc. 8.
- Marija Šebjan Pušenjak, B. Sc. 9.
- 10. Marjeta Trobec, M. Sc.

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- Ivana Marušić, Visoka tehnična šola Oddelek za mehatroniko, Bjelovar, Croatia, 5. 21.-22. 3. 2018
- 6. Ivan Seković, Visoka tehnična šola - Oddelek za računalništvo, Bjelovar, Croatia, 21.-22. 3. 2018
- Ivana Jurković, Visoka tehnična šola, Bjelovar, Croatia, 21.-22. 3. 2018 7
- Jon Wulf Petersen, Plougmann Vingtoft, Copenhagen, Denmark, 11. 10. 2018 8 9.
- Brecht Vanlerberghe, Bio Base Europe Pilot Plant, Gent, Belgium, 11. 10. 2018

#### Technical and administrative staff

- 11. Barbara Bercko, B. Sc., left 01.06.18
- 12. Maja Ivanišin, M. Sc.
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- Tomaž Lutman, B. Sc. 15.
- 16. David Mirosavljević, B. Sc., left 01.11.18
- 17. Matej Mrak, B. Sc.
- 18. Urška Mrgole, B. Sc.
- 19. Nataša Požarnik, B. Sc.
- 20. Robert Premk, B. Sc.
- 21. Luka Virag, B. Sc., 01.02.18, transferred to Department U2

### PUBLISHED CONFERENCE CONTRIBUTION

1. Urška Mrgole, Špela Stres, "Promotion of the STEM disciplines among youth", In: Uroš Rajkovič (ed.), Andrej Brodnik (ed.), Education in information society: conference proceedings, Ljubljana, 2018, 152-155.

### PROFESSIONAL MONOGRAPH

1. Špela Stres, Levin Pal, Priročnik o prenosu tehnologij: za slovensko gospodarstvo in slovensko znanost, Ljubljana: Center za prenos tehnologij in inovacij na Institutu Jožef Stefan, 2018.

# **CENTER FOR SMART CITIES** AND COMMUNITIES

# CSC&C

The Center for Smart Cities and Communities CSC&C was established at the beginning of 2017. The main task of the center is to coordinate and operate the Strategic Development and Innovation Partnership of Smart Cities and Communities (SRIP SC&C). In addition, the center also promotes cross-sectoral cooperation within the Jožef Stefan Institute, thus supporting partnerships in state-of-the-art technologies and at the same time actively participating in the creation of national **R&D** policies for the coming years.

### Strategic Development Innovation Partnership Smart Cities and Communities

The Strategic Development Innovation Partnership Smart Cities and Communities is a form of partnership in which stakeholders have joined forces in developing and selling solutions to improve the quality of life in the cities of the future.

The purpose of SRIP SC&C is to connect companies and research institutions in a particular field into value chains, to set priorities for development investments and to coordinate R&D activities. We are building a good support Head: environment for sharing knowledge and experiences in the form of workshops, seminars and joint events; we offer Matjaž Šteblaj, B. Sc. access to test environments, laboratories, databases; and we provide assistance in market analysis, human-resources development, intellectual-property protection and internationalization.

We want to approach the smaller towns in Central and Eastern Europe with solutions, as we consider that because of its size and geostrategic position, Slovenia is very suitable as a reference country for various "smart urban" solutions suitable for implementation in other parts of Central and Eastern Europe.

The SRIP SC&C was formally constituted at the Assembly on 23 March 2017, and currently involves more than 140 companies and research institutions from all over Slovenia.

### Key areas and technologies

The Strategic Research and Innovation Partnership Smart Cities and Communities covers several research areas as well as the ICT horizontal key enabling technologies (Figure 1).

#### The key objectives of SRIP SC&C are:

Developing globally competitive solutions in the field of SC&C, Establishment of a globally recognized ecosystem of partners that permanently and synergistically build and link their competencies in SC&S domains and technologies,

Providing resources and conditions (an open-platform ecosystem) for as short a time as possible from planning to marketing globally competitive high-tech solutions,

International promotion of the Slovenian "brand" in Smart Town and Community - Smart Towns.

The SRIP SC&C creates and supports business and research synergies in smart cities for new products, services and technologies, and helps companies enter the global market by focusing on niche areas, with the aim of making Slovenian companies an important European provider of such solutions.

In April 2018 we signed an agreement with the Ministry of Economy and Technology to co-finance Phase 2 of the "Strategic Development Innovation Partnership in the Smart Cities and Communities" operation, which confirms the SRIP PMiS guidelines set out in the Action Documents.

We organized several free workshops and seminars for SRIP PMiS members: Workshop Promoting the Implementation of Research and Development Projects (TRL3-6), 22. 01. 2018; Workshop on the preparation of the project for the public tender MGRT TRL 6-9, 12. 04. 2018; Workshop on Intellectual Property, 14. 05. 2018; Seminar on Private Sector Involvement in EU External Financial Instruments, 1. 06. 2018; SRIP PMiS Members Meeting, 04. 07. 2018; Workshop Presentation of the DEMO PILOTS II 2018 Call at the IJS, 30. 08. 2018; Workshop on Technology Breakthroughs and Good Practices, 22. 11. 2018.

The SRIP PMIS actively participated in and promoted itself at some major events in Slovenia: National Conference on the Internationalization of the Slovenian Economy; 06. 04. 2018, Brdo pri Kranju; Webinar Partnership for Electric (r) evolution, 23. 04. 2018; Bass Conference at Brdo pri Kranju, 25. 04. 2018; Energy transition as an opportunity for the Slovenian economy on 26.04.2018 at the Chamber of Commerce and Industry; Practical Tips

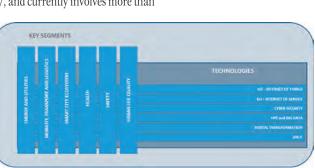


Figure 1: Key areas and technologies



for Writing a Competitive and Successful Project Proposal, 23. 05. 2018; 10th ICT Industrial Forum, 04. 06. 2018 in Portorož; AGRA Fair in Gornja Radgona on 26. 08. 2018; Conference: Urban Innovation in the Local Environment; 28. 09. 2018 in Murska Sobota; 2nd Congress of Slovenian Municipalities in Rimske Toplice , 03. 10. 2018 organized by SOS (Community of Municipalities of Slovenia), ZOS (Association of Municipalities of Slovenia), ZMOS (Association of Urban Municipalities of Slovenia) and the Institute of Public Services; Presentation of the functioning of the SRIP PMIS as part of the 27th Forum of Excellence and Mastery in Trebnje, 03. 10. 2018; 26th International Conference on Materials and Technologies: Consultation: Developing Competencies for Future Challenges, 04. 10. 2018, Portorož, GH Bernardin; Love Digital; 22.-23. 10 2018: Development of competences for digitization of Slovenian companies; 3. New Year's meeting with researchers in Maribor, 14. 12. 2018; GreenTech Forum Bled 2018: Green Economy Challenges; 12. 09. 2018; Bled Strategic Forum International Consultation & Accompanying Event; Celje International Trade Fair (MOS 2018).

As part of **the promotion and internationalization** of the SRIP PMiS, many activities for members took place. The SRIP PMiS Director attended the Open & Agile Smart Cities Workshop in Brussels. As part of the event, he had discussions with city representatives and service providers, who presented themselves at the workshop. The Director of the SRIP PMiS attended a meeting with Ms. Isabelle Du Sutter, a representative of the French Competence Center in the field of Systematic Paris Region Digital Ecosystem, who visited the Jožef Stefan Institute. He presented to her the purpose and operation of the SRIP PMiS. The conversation identified an interest in participating.

## STAFF

Technical and administrative staff

1. Dr. Nevenka Cukjati

2. Petja Grizilo, B. Sc.

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

- 1. Strategic Research & Innovation Partnership (SRIP) Smart Cities and Communities Matjaž Šteblaj, B. Sc.
- Ministry of Economic Development and Technology 2. Strategic Research & Innovation Partnership Factories of the Future (SRIP SC&C) Dr. Nevenka Cukiati

Ministry of Economic Development and Technology

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- 1. Csaba Hegedűs, Paolo Ciancarini, Attila Frankó, Aleš Kancilija, István Moldován, Gregor Papa, Špela Poklukar, Mario Riccardi, Alberto Sillitti, Pal Varga, "Proactive maintenance of railway switches", In: 5th International Conference on Control, Decision and Information Technologies, CoDlt 2018, April 10.13, 2018, Thessaloniki, Greece: conference digest, 2018, 725-730.
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- Rok Hribar, Jurij Šilc, Gregor Papa, "Construction of Heuristic for Protein Structure Optimization using deep reinforcement learning", In: Peter Korošec (ed.), Nouredine Melab (ed.), El-Ghazali Talbi (ed.),

- 3. Nataša Juvančič, B. Sc., left 06.03.18
- 4. Martin Pečar, B. Sc., Head, left 03.01.18
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- SRIP (Strategic Research & Innovation Partnership) Smart Cities and Communities Dr. Nevenka Cukjati

Bioinspired optimization methods and their applications: 8th International Conference, BIOMA 2018 Paris, France, May 16-18, 2018: proceedings, (Lecture notes in computer science **10835**), 2018, 151-162.

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# **CENTER FACTORY** OF THE FUTURE

# **CFoF**

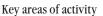
Center Factories of the Future - CToP, run by Rudi Panjtar, was established in early 2017. The main task of the newly established center is to coordinate and operate the Strategic Development and Innovation Partnership of Factory of the Future (SRIP ToP). In addition, the center also encourages cross-sectoral cooperation within the Jozef Stefan Institute, thereby contributing to the support of the latest technology partnership and at the same time actively participating in the development of R&D policies in the future.

#### What does the Factory of the Future Strategic Development Innovation Partnership offer?

The SRIP Factory of the Future (SRIP ToP) strategy is to gather and integrate Slovenian research and innovation knowledge and experience in the industrial and academic spheres and highlight the priority breakthroughs of new products, technologies and services for Factories of the Future. We have established a supportive environment with expert services for industry and research organizations, with an emphasis on developing new cutting-edge technologies that combine and build on existing Slovenian research and innovation achievements.

SRIP ToP creates and supports business and research synergies in the area of future factories for new products, Rudi Panjtar, B. Sc. services and technologies, and helps businesses enter the global market by focusing on niche areas.

The 90 members of SRIP ToP come from various companies, associations or institutions from Slovenia. The operation of SRIP ToP focuses on the greater integration of knowledge and the joint appearance of stakeholders in domestic and foreign markets. The primary goals are to increase the share of high-tech industrial products in exports and to increase the added value of Slovenian industry.



The SRIP Factories of the Future includes eight areas (verticals), and horizontal networks with key technologies are interwoven through all (Figure 1).

By effectively directing R&D and introducing knowledge and technologies that enable the production of higher-quality products, reducing energy and raw materials, reducing environmental pollution, improving human

involvement, etc., SRIP ToP also indirectly contributes to accelerating the transition to a low-energy, energyefficient economy, and reduced greenhouse-gas emissions. This is in order to intensively promote the transition to a low-carbon society and to a circular economy. The essence of the concept of factories of the future is mainly reflected in the greater potential for reuse of raw materials, made possible by more flexible and optimally managed production.

At the end of 2017, we moved to phase 2 of the call for strategic development innovation partnerships. We have prepared an activity plan for individual areas of work and shared services. We have established four beneficiaries, who independently implement their business plan within their own clusters and define the relationships between

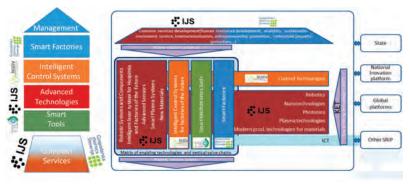


Figure 1: Scheme of SRIP ToP domains

them, ensuring the outward unified functioning of SRIP ToP, while allowing beneficiaries a great deal of autonomy in their decisions. We also unanimously adopted the Regulation on Financing the SRIP ToP Business Model, which defined the financial relationships between the beneficiaries.

In the field of internationalization, we have become full members of EFFRA, the EU umbrella for the Factories of the Future. In the area of S3, we took over the co-leadership of Artificial Intelligence in Production (AI & HMI), and through the Greenomed, BoifoksAlps, SmartSpace projects within Ljubljana Technology Park, we worked with various stakeholders of regions, involved in the Vanguard Initiative. Together with the Ministry of Foreign Affairs we also realized the visit and presentation of our members in Denmark (Odense) and participated in the fair's activities.

As part of the Bifoks Alps project, we also attended an Industry 4.0 fair in Molhouse, France, together with our members.



As part of the preparation of the Action Plan and in order to promote networking, the exchange of information and to encourage organizations to become members of SRIP ToP, in 2018 we conducted SRIP ToP demonstration events (among the most notable were the EU Robotics Days 2018, Nanotechnology Presentation Day, ToP and Industry Challenge, Introduction of MGRT calls, Vanguard Workshop, and Tetramax Workshops). We organized various thematic workshops around Slovenia and co-organized high-profile conferences (Midem 2018, Best Practice Day, Plasma and Vacuum Technology, Service and Assembly Automation Consultation 2018 - ASM, 18, Toolmaking Day 2018).

We actively participated in major events in Slovenia and abroad, to name a few: Greenomed-First Political Meeting, Agra Fair in Gornja Radgona, SRIP ToP Presentation for Project Evaluators, Kočevje Workshop 4.0 in Kočevje, Startup Conference and Technology Transfer at Ljubljana Technology Park.

In December 2018 we joined the Panoramed Interreg Mediteran project as a co-lead of the work package innovation.

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# **R&D GRANTS AND CONTRACTS**

- Strategic Research & Innovation Partnership Factories of the Future (SRIP FoF) 1. Rudi Panjtar, B. Sc. Ministry of Economic Development and Technology
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Ministry of Economic Development and Technology

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- FoF Factories of the Future, Centre FoF SRIP 3.
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