











Annual Report 2013







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INTRODUCTION



Prof. Jadran Lenarčič, Director of the Jožef Stefan Institute

This year, like every other year, I look at the annual report of the Jožef Stefan Institute with great pleasure and pride. I am delighted by the achievements of our researchers who, in spite of the worsening conditions, achieved the highest rankings in certain fields.

Unfortunately, the socio-political climate in our country is not in favour of incorporating scientific research into economic and social development on a scale and in a form needed for Slovenia to go from "fire fighting" to planned, systematic development in all key areas.

Furthermore, development issues connected to scientific research do not become the focus of socio-political debate, even in a pre-election period. For this reason, Slovenia is not so successful at profiting from research achievements in practice and developing its economic position. It is paradoxical that the state is not giving any attention to crucial development issues. The main focus is still on even greater regulation of society, which is a counterproductive measure because it suffocates the creativity and initiative of individuals and institutions.

The result is that in Slovenia the role of scientific research is even less important and there is even greater ignorance of the processes that lead to scientific discoveries as well as the processes involved in transforming a scientific achievement, a new product, a new technology, a new creation, into something with commercial and economic value. Research is seen by the authorities as just an item in the budget that needs to be cut.

In the past two years the Jožef Stefan Institute has reacted to the cuts in government funding by increasing its income from the EU and from external partners. This is the main reason why we have managed to keep our doors open for young people. I am aware of the risks of this strategy, but it is worthy of the name of our 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 build a Physics Institute

1949

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

1952

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

1954

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

1956

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

1958

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

1959

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



Mass spectrometer at the JSI (about 1960)

1962

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

1966

Nuclear research reactor TRIGA starts operation

1968

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

1969

Institute is renamed as the Jožef Stefan Institute

1970

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

1971

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



Institute buildings after the opening in 1953

1972

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

1974

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

1976

First Yugoslav 8-bit processor computer DARTA 80

1979

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

1982

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

1983

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



The Reactor Centre, Podgorica, built in 1966

1985

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

1987

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



Nuclear magnetic resonance spectrometer

1989

 \sim Milan Čopič Nuclear Training Centre established 1990

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

1995

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

1999

~ Jožef Stefan Institute celebrates its 50th anniversary

2003

 \sim Jožef Stefan International Postgraduate School established

2004

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

2007

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



The beginnings of robotics at the JSI, in 1985

FORMER DIRECTORS



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

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

ORGANISATION OF THE JOŽEF STEFAN INSTITUTE

BOARD OF GOVERNORS

DIRECTOR

SCIENTIFIC COUNCIL

RESEARCH DEPARTMENTS

Physics

Theoretical Physics (F-1) Prof. Svjetlana Fajfer Low and Medium Energy Physics (F-2) Asst. Prof. Primož Pelicon Thin Films and Surfaces (F-3) Dr. Peter Panjan, 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. Andrej Trkov **Experimental Particle Physics (F-9)** Prof. Marko Mikuž

Chemistry and Biochemistry

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

Electronics and Information Technology

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

Reactor Techniques and Energetics

Reactor Engineering (R-4) Prof. Leon Cizelj

CENTRES

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

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

ADMINISTRATION, SERVICES AND SUPPORT UNITS

Administration and Services

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

Support Units

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

PARTICIPATION IN THE REGIONAL DEVELOPMENT OF RESEARCH

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

MANAGEMENT

DIRECTORATE

Director JSI Prof. Jadran Lenarčič

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

BOARD OF GOVERNORS

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STAFF QUALIFICATIONS

1949-2013



RECIPIENTS OF THE JSI AWARDS AND TITLES

HONORARY MEMBERS

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

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

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

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

Prof. Milan Osredkar[‡], Director of the Jožef Stefan Institute from 1963 to 1975 (1919-2003) Prof. Anton Peterlin[‡], Founder and First Director of the Jožef Stefan Institute from

1949 to 1955 (1908 - 1993)

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

INTERNATIONAL COOPERATION

Multilateral international cooperation	No. of projects
7. FP (COOPERATION: HEALTH, FOOD, AGRICULTURE/FISHERIES, BIOTECHNOLOGY, INFORMATION COMMUNICATION TECHNOLOGIES, NANOSCIENCES + NANOTECHNOLOGIES, MATERIALS + NEW PRODUCTION TECHNOLOGIES, ENERGY, ENVIRONMENT AND CLIMATE CHANGE,	117
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)	
7. FP - EURATOM	35
ESRR	16
OTHERS (COST, IAEA, EIE, IRMM, ESA, NATO, CIP, CE, SEE, EMRP, WHO, LIFE+, ARTEMIS)	178
ΤΟΤΑΙ	246

Bilateral cooperation	No. of projects
Argentine	3
Belgium	1
Brazil	1
China	5
Montenegro	3
Cyprus	1
France	19
Croatia	7
Italy	2

Bilateral cooperation	No. of projects
Japan	7
Korea	1
Macedonia	1
Romania	4
Russia	2
Serbia	5
Turkey	1
Ukraine	4
USA	18
TOTAL	85

INTERNATIONAL COOPERATION AGREEMENTS

In 2013, cooperation agreements were signed between the Jožef Stefan Institute and:

- 1. Los Alamos National Laboratory (LANL), Los Alamos; Sandia National Laboratories (SNL), USA (F1)
- 2. Stichting INCAS, Assen, The Netherlands (F2)
- 3. Harder Ditial Sova a.d., Niš, Serbia (F4)
- 4. Institute of Electronic Materials Technology, Warsaw, Poland (F5)
- 5. Kimberly-Clark Europe Limited, Surrey, Great Britain (F5)
- Westinghouse Electric Sweden AB, Vasteras, Sweden; Westinghouse Electric Company LLC, Pennsylvania, USA (F8)
- 7. The United Kingdom Atomic Energy Authority (CCFE) of Culham Science Centre, Abingdon, Oxfordshire, United Kingdom, (F8)
- Los Alamos National Security, LLC, Los Alamos National Laboratory, Technology Transfer Division, Los Alamos, NM, USA (F8)
- 9. The Centre National de la Recherche Scientifique, Paris, France (B2)
- 10. VIB vzw, Zwijnaarde, Belgium (B2)

- 11. University of Milan, Milan, Italy (B2)
- 12. Institute of Metrology of Bosnia and Herzegovina, Sarajevo, Bosnia and Herzegovina (O2)
- 13. Al-Farabi Kazakh National University, Almaty, Kazakhstan (O2)
- 14. State Ecological Academy of Postgraduate Education and Management, Kiev, Ukraine (O2)
- 15. The Foundation INCAS3, Assen, The Netherlands (E6, E9)
- 16. GainSpan Corporation, San Jose, CA, USA (E7)
- 17. Johannes Gutenberg University Mainz, Mainz, Germany (RIC)
- 18. Knowledge 4 All Foundation Ltd., London, United Kingdom (CT3)
- 19. Fish & Richardson P. C., Minneapolis, Minnesota, USA (CTT)
- 20. Bastille LLC, Memphis, TN, USA (CTT)
- 21. Goodyear S.A., Colmar-Berg, Luxembourg (CTT)

COOPERATION WITH UNIVERSITIES

FULL-TIME FACULTY MEMBERS

Professors

- 1. Asst. Prof. Denis Arčon, University of Ljubljana, Faculty of Mathematics and Physics
- 2. Prof. Iztok Arčon, University of Nova Gorica
- 3. Prof. Janez Bonča, University of Ljubljana, Faculty of Mathematics and Physics
- 4. **Prof. Ivan Bratko**, Academician, University of Ljubljana, Faculty of Computer and Information Science
- 5. Prof. Milan Brumen, University of Maribor, Faculty of Education
- 6. Prof. Dean Cvetko, University of Ljubljana, Faculty of Mathematics and Physics
- 7. Prof. Mojca Čepič, University of Ljubljana, Faculty of Education
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- 11. Prof. Svjetlana Fajfer, University of Ljubljana, Faculty of Mathematics and Physics
- 12. Prof. Bojan Golli, University of Ljubljana, Faculty of Education
- 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. Borut Paul Kerševan, University of Ljubljana, Faculty of Mathematics and Physics
- 17. Prof. Igor Klep, University of Ljubljana, Faculty of Mathematics and Physics
- 18. Prof. Juš Kocijan, University of Nova Gorica
- 19. Prof. Gregor Cigler, University of Ljubljana, Faculty of Mathematics and Physics
- 20. Asst. Prof. Samo Korpar, University of Maribor, Faculty of Chemistry and Chemical Engineering
- 21. Prof. Janko Kos, University of Ljubljana, Faculty of Pharmacy
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- 23. Prof. Samo Kralj, University of Maribor, Faculty of Education
- Prof. Edvard Kramar, University of Ljubljana, Faculty of Mathematics and Physics
 Prof. Marjeta Kramar Fijavž, University of Ljubljana, Faculty of Mathematics
- and Physics
- 26. **Prof. Peter Križan**, University of Ljubljana, Faculty of Mathematics and Physics
- 27. **Prof. Brigita Lenarčič**, University of Ljubljana, Faculty of Chemistry and Chemical Technology
- 28. Prof. Andrej Likar, University of Ljubljana, Faculty of Mathematics and Physics
- 29. Prof. Marko Mikuž, University of Ljubljana, Faculty of Mathematics and Physics
- 30. Prof. Igor Muševič, University of Ljubljana, Faculty of Mathematics and Physics
- 31. Prof. Rudolf Podgornik, University of Ljubljana, Faculty of Mathematics and Physics
- 32. Asst. Prof. Tomaž Podobnik, University of Ljubljana, Faculty of Mathematics
- and Physics 33. Prof. Peter Prelovšek, University of Ljubljana, Faculty of Mathematics and Physics
- 34. **Asst. Prof. Saša Prelovšek Komelj**, University of Ljubljana, Faculty of Mathematics and Physics
- 35. Prof. Anton Ramšak, University of Ljubljana, Faculty of Mathematics and Physics

- 36. Asst. Prof. Iztok Savnik, University of Primorska, Faculty of Mathematics, Natural Sciences and Information Technologies
- 37. Prof. Janez Seliger, University of Ljubljana, Faculty of Mathematics and Physics
- Prof. John Shawe-Taylor, University College London, Centre for Computational Statistics and Machine Learning
- 39. Prof. Janez Stepišnik, University of Ljubljana, Faculty of Mathematics and Physics
- 40. Prof. Saša Svetina, Academician, University of Ljubljana, Faculty of Medicine
- 41. Prof. Simon Širca, University of Ljubljana, Faculty of Mathematics and Physics
- 42. Prof. Žiga Šmit, University of Ljubljana, Faculty of Mathematics and Physics
- 43. Prof. Borut Štrukelj, University of Ljubljana, Faculty of Pharmacy
- 44. **Prof. Jurij Franc Tasič**, University of Ljubljana, Faculty of Electrical Engineering, University of Primorska, Koper
- 45. Asst. Prof. Tanja Urbančič, University of Nova Gorica
- 46. Asst. Prof. Nataša Vaupotič, University of Maribor, Faculty of Education
- 47. Prof. Danilo Zavrtanik, University of Nova Gorica
- 48. Prof. Marko Zgonik, University of Ljubljana, Faculty of Mathematics and Physics
- 49. Asst. Prof. Primož Ziherl, University of Ljubljana, Faculty of Mathematics and Physics
- 50. Prof. Slobodan Žumer, University of Ljubljana, Faculty of Mathematics and Physics

Assistants and researchers

- 1. Asst. Prof. Marko Bračko, University of Maribor, Faculty of Chemistry and Chemical Engineering
- 2. Dr. Gregor Cigler, University of Ljubljana, Faculty of Mathematics and Physics
- 3. Dr. Jure Leskovec, Stanford University, Palo Alto, California, USA
- 4. Dr. Tomaž Rejec, University of Ljubljana, Faculty of Mathematics and Physics

PART-TIME FACULTY MEMBERS

Professors

- 1. Asst. Prof. Andreja Benčan Golob, Jožef Stefan International Postgraduate School, Ljubljana
- 2. Asst. Prof. Ljudmila Benedik, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Faculty of Mathematics and Physics and Jožef Stefan International Postgraduate School, Ljubljana
- 3. Asst. Prof. Aleš Berlec, University of Ljubljana, Faculty of Pharmacy
- 4. Asst. Prof. Slavko Bernik, Jožef Stefan International Postgraduate School, Ljubljana
- 5. Asst. Prof. Anton Biasizzo, Jožef Stefan International Postgraduate School, Ljubljana
- 6. Asst. Prof. Vid Bobnar, Jožef Stefan International Postgraduate School, Ljubljana
- 7. **Prof. Marko Bohanec**, University of Nova Gorica, School of Enginnering and Management and Jožef Stefan International Postgraduate School, Ljubljana
- 8. **Prof. Vladimir Cindro**, University of Ljubljana, Faculty of Natural Sciences and Technology
- 9. Prof. Leon Cizelj, University of Ljubljana, Faculty of Mathematics and Physics
- 10. Asst. Prof. Uroš Cvelbar, Jožef Stefan International Postgraduate School, Ljubljana
- 11. **Prof. Miran Čeh**, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Jožef Stefan International Postgraduate School, Ljubljana
- 12. Asst. Prof. Nina Daneu, Jožef Stefan International Postgraduate School, Ljubljana

- Prof. Marko Debeljak, Jožef Stefan International Postgraduate School, Ljubljana, University of Ljubljana, University of Primorska, University of Nova Gorica, University of Tennessee, USA, University of Lorain, France
- 14. Asst. Prof. Goran Dražič, Jožef Stefan International Postgraduate School, Ljubljana
- 15. **Prof. Sašo Džeroski**, University of Maastricht, The Netherlands and Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Borka Džonova Jerman Blažič, University of Ljubljana, Faculty of Economics and Jožef Stefan International Postgraduate School, Ljubljana
- 17. Asst. Prof. Tomaž Erjavec, Jožef Stefan International Postgraduate School, Ljubljana
- Asst. Prof. Ingrid Falnoga, University of Ljubljana, Faculty of Maritime Studies and Transport
- 19. Asst. Prof. Andrej Filipčič, University of Nova Gorica
- 20. **Prof. Bogdan Filipič**, University of Ljubljana, Faculty of Computer and Information Science, University of Nova Gorica, Faculty of Engineering and Management, Jožef Stefan International Postgraduate School, Ljubljana
- 21. Asst. Prof. Marko Fonović, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Matjaž Gams, University of Ljubljana, Faculty of Computer and Information Science, Jožef Stefan International Postgraduate School, Ljubljana
- 23. Asst. Prof. Marko Gerbec, Jožef Stefan International Postgraduate School, Ljubljana
- 24. Prof. Ester Heath, Jožef Stefan International Postgraduate School, Ljubljana
- 25. **Prof. Milena Horvat**, Jožef Stefan International Postgraduate School, Ljubljana, University of Maribor, Faculty of Mechanical Engineering
- 26. Asst. Prof. Marko Hrovat, Jožef Stefan International Postgraduate School, Ljubljana
- 27. Asst. Prof. Jernej Iskra, Jožef Stefan International Postgraduate School, Ljubljana and University of Maribor, Faculty of Chemistry and Chemical Engineering
- 28. Asst. Prof. Boštjan Jančar, Jožef Stefan International Postgraduate School, Ljubljana
- 29. Asst. Prof. Tomaž Javornik, Jožef Stefan International Postgraduate School, Ljubljana
- 30. Asst. Prof. Robert Jeraj, University of Ljubljana, Faculty of Mathematics and Physics, University of Wisconsin, School of Medical Physic, Madison
- 31. Asst. Prof. Zvonka Jeran, Jožef Stefan International Postgraduate School, Ljubljana
- 32. Prof. Đani Juričić, University of Nova Gorica, School of Environmental Sciences, University of Maribor, Faculty of Logistics and Jožef Stefan International Postgraduate School, Ljubljana
- 33. Prof. Viktor Kabanov, Jožef Stefan International Postgraduate School, Ljubljana
- 34. **Prof. Gorazd Kandus**, University of Maribor, Faculty of Electrical Engineering and Computer Science and Jožef Stefan International Postgraduate School, Ljubljana
- 35. **Prof. Monika Kapus Kolar**, University of Maribor, Faculty of Electrical Engineering and Computer Science
- 36. Asst. Prof. Ivo Kljenak, University of Ljubljana, Faculty of Mathematics and Physics
- 37. Asst. Prof. Tomaž Klobučar, Jožef Stefan International Postgraduate School, Ljubljana, DOBA Faculty of Applied Business and Social Studies, Maribor
- Prof. Spomenka Kobe, University of Ljubljana, Faculty of Natural Sciences and Technology, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Juš Kocijan, University of Nova Gorica, School of Engineering and Management and Jožef Stefan International Postgraduate School, Ljubljana
- 40. Asst. Prof. Robert Kocjančič, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Ivan Aleksander Kodeli, University of Maribor, Faculty of Energy Technology
- 42. Asst. Prof. Matej Andrej Komelj, University of Ljubljana, Faculty of Mathematics and Physics
- 43. Prof. Branko Kontić, University of Nova Gorica
- 44. Asst. Prof. Dušan Kordiš, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Peter Korošec, University of Primorska, Koper, Faculty of Mathematics, Sciences and Information Technologies

- 46. Asst. Prof. Barbara Koroušić Seljak, Jožef Stefan International Postgraduate School
- Prof. Tomaž Kosmač, University of Ljubljana, Faculty of Natural Sciences and Technology, Medical Faculty and Jožef Stefan International Postgraduate School, Ljubljana
- 48. Dr. Igor Kovač, Fachhochschule Joaneum, Graz, Austria
- 49. Asst. Prof. Janez Kovač, University of Ljubljana, Faculty of Natural Sciences and Technology and Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Igor Križaj, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Biotechnical Faculty, Medical Faculty, Jožef Stefan International Postgraduate School, Ljubljana
- 51. Asst. Prof. Danjela Kuščer Hrovatin, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Zdravko Kutnjak, University of Ljubljana, Faculty of Mathematics and Physics and Faculty of Mechanical Engineering, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Nada Lavrač, University of Nova Gorica, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Jadran Lenarčič, University of Ljubljana, Faculty of Electrical Engineering, University of Nova Gorica, Università degli studi di Bologna
- 55. Asst. Prof. Matej Lipoglavšek, University of Ljubljana, Faculty of Mathematics and Physics
- 56. Asst. Prof. Darja Lisjak, Jožef Stefan International Postgraduate School, Ljubljana
- 57. Prof. Sonja Lojen, University of Nova Gorica, School of Environmental Sciences
- Prof. Boris Majaron, University of Ljubljana, Faculty of Mathematics and Physics
- Prof. Darko Makovec, University of Maribor, Faculty of Chemistry and Chemical Engineering and Faculty of Medicine, Jožef Stefan International Postgraduate School, Ljubljana
- 60. Prof. Barbara Malič, Jožef Stefan International Postgraduate School, Ljubljana
- 61. Asst. Prof. Igor Mandić, University of Ljubljana, Faculty of Natural Sciences and Technology
- 62. Prof. Borut Mavko, University of Ljubljana, Faculty of Mathematics and Physics
- 63. Asst. Prof. Paul McGuiness, Jožef Stefan International Postgraduate School, Ljubljana
- 64. **Prof. Igor Mekjavić**, University of Portsmouth, Institute of Biomedical and Biomolecular Sciences, Portsmouth, United Kingdom
- 65. Asst. Prof. Alenka Mertelj, University of Ljubljana, Faculty of Mathematics and Physics
- 66. Asst. Prof. Tomaž Mertelj, University of Ljubljana, Faculty of Mathematics and Physics
- Prof. Dragan Dragoljub Mihailović, University of Ljubljana, Faculty of Mathematics and Physics and Jožef Stefan International Postgraduate School, Ljubljana
- 68. Prof. Radmila Milačič, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Ingrid Milošev, University of Zagreb, Croatia, Faculty of Chemical Engineering and Technology and Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Dunja Mladenić, Jožef Stefan International Postgraduate School, Ljubljana and University of Zagreb, Croatia, University of Ljubljana, Faculty of Education, University of Nova Gorica, University of Primorska, Koper
- 71. Asst. Prof. Mihael Mohorčič, Jožef Stefan International Postgraduate School, Ljubljana
- 72. **Prof. Miran Mozetič**, University of Nova Gorica, Jožef Stefan International Postgraduate School, Ljubljana, University of Ljubljana, Faculty of Natural Sciences and Technology
- 73. Asst. Prof. Bojan Nemec, Jožef Stefan International Postgraduate School, Ljubljana
- 74. **Prof. Franc Novak**, University of Maribor, Faculty of Electrical Engineering and Computer Science and Jožef Stefan International Postgraduate School, Ljubljana
- 75. Asst. Prof. Roman Novak, Jožef Stefan International Postgraduate School, Ljubljana
- 76. Asst. Prof. Saša Novak Krmpotič, Jožef Stefan International Postgraduate School, Ljubljana

- 77. Prof. Nives Ogrinc, Jožef Stefan International Postgraduate School, Ljubljana
- 78. Asst. Prof. Gregor Papa, Jožef Stefan International Postgraduate School, Ljubljana
- 79. Asst. Prof. Primož Pelicon, University of Ljubljana, Faculty of Mathematics and Physics
- 80. Asst. Prof. Toni Petan, University of Nova Gorica, School of Environmental Sciences, School for Viticulture and Enology
- 81. Asst. Prof. Uroš Petrovič, University of Nova Gorica, School of Environmental Sciences, School for Viticulture and Enology
- 82. Asst. Prof. Maja Ponikvar-Svet, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Jože Pungerčar, University of Ljubljana, Faculty of Chemistry and Chemical Technology
- Asst. Prof. Aleksander Rečnik, University of Ljubljana, Faculty of Natural Sciences and Technology, Jožef Stefan International Postgraduate School, Ljubljana
- 85. Prof. Maja Remškar, Jožef Stefan International Postgraduate School, Ljubljana
- 86. **Prof. Boris Rogelj**, University of Ljubljana, Faculty of Chemistry and Chemical Technology
- 87. Asst. Prof. Igor Serša, University of Ljubljana, Faculty of Natural Sciences and Technology, Jožef Stefan International Postgraduate School, Ljubljana
- 88. Asst. Prof. Tomaž Skapin, Jožef Stefan International Postgraduate School
- 89. Prof. Borut Smodiš, University of Ljubljana, Faculty of Chemistry and Chemical Technology, University of Maribor, Faculty of Energy technology, University of Nova Gorica, School of Environmental Sciences and Jožef Stefan International Postgraduate School, Ljubljana
- 90. Prof. Marko Starič, University of Ljubljana, Faculty of Mathematics and Physics
- 91. Prof. Stojan Stavber, Jožef Stefan International Postgraduate School, Ljubljana
- 92. **Prof. Vekoslava Stibilj**, Jožef Stefan International Postgraduate School, Ljubljana
- 93. Prof. Veronika Stoka, Jožef Stefan International Postgraduate School, Ljubljana
- 94. **Prof. Stanislav Strmčnik**, University of Nova Gorica, School of Engineering and Management
- 95. **Prof. Danilo Suvorov**, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Mathematics and Physics, Jožef Stefan International Postgraduate School, Ljubljana
- 96. Prof. Janez Ščančar, Jožef Stefan International Postgraduate School, Ljubljana
- 97. Asst. Prof. Jurij Šilc, Jožef Stefan International Postgraduate School, Ljubljana
- 98. Asst. Prof. Srečo Davor Škapin, Jožef Stefan International Postgraduate School, Ljubljana
- 99. Asst. Prof. Zdenka Šlejkovec, Jožef Stefan International Postgraduate School, Ljubljana
- 100. Asst. Prof. Janez Štrancar, Jožef Stefan International Postgraduate School, Ljubljana
- 101. Asst. Prof. Sašo Šturm, Jožef Stefan International Postgraduate School, Ljubljana
- 102. Asst. Prof. Aleš Švigelj, Jožef Stefan International Postgraduate School, Ljubljana
- 103. Prof. Iztok Tiselj, University of Ljubljana, Faculty of Mathematics and Physics
- 104. Asst. Prof. Andrej Trkov, University of Ljubljana, Faculty of Mathematics and Physics and University of Maribor, Faculty of Energy Technology
- 105. Asst. Prof. Roman Trobec, University of Ljubljana, Faculty of Computer and Information Science
- 106. Prof. Boris Turk, University of Ljubljana, Biotechnical Faculty, Faculty of Chemistry and Chemical Technology, Jožef Stefan International Postgraduate School, Ljubljana
- Prof. Dušan Turk, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Medicine, Jožef Stefan International Postgraduate School, Ljubljana
- 108. **Prof. Vito Turk**, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Jožef Stefan International Postgraduate School, Ljubljana
- 109. Asst. Prof. Aleš Ude, Jožef Stefan International Postgraduate School, Ljubljana
- 110. Prof. Janja Vaupotič, University of Ljubljana, Faculty of Medicine, University of

Nova Gorica and Jožef Stefan International Postgraduate School, Ljubljana

- 111. Asst. Prof. Alenka Vesel, Jožef Stefan International Postgraduate School
- 112. Asst. Prof. Damir Vrančić, Jožef Stefan International Postgraduate School and University of Maribor, Faculty of Logistics
- Prof. Boštjan Zalar, University of Ljubljana, Faculty of Mathematics and Physics and Biotechnical Faculty, Jožef Stefan International Postgraduate School, Ljubljana
- 114. Prof. Marko Zavrtanik, University of Nova Gorica
- 115. Prof. Aleksander Zidanšek, University of Maribor, Faculty of Education, Jožef Stefan International Postgraduate School, Ljubljana
- 116. Prof. Eva Žerovnik, Jožef Stefan International Postgraduate School, Ljubljana
- 117. Asst. Prof. Matjaž Žitnik, University of Ljubljana, Faculty of Mathematics and Physics
- 118. Asst. Prof. Leon Žlajpah, Jožef Stefan International Postgraduate School, Ljubljana
- 119. Asst. Prof. Bernard Ženko, Faculty of Information Studies, Novo Mesto
- 120. Asst. Prof. Martin Žnidaršič, Faculty of Information Studies, Novo Mesto

Assistants and researchers

- Dr. Tanja Arh, Jožef Stefan International Postgraduate School, Ljubljana, DOBA Faculty of Applied Business and Social Studies, Maribor
- 2. Dr. Zoran Arsov, University of Ljubljana, Faculty of Mathematics and Physics
- 3. Dr. Jan Babič, University of Ljubljana, Faculty of Electrical Engineering
- 4. Dr. Klemen Bučar, University of Ljubljana, Faculty of Mathematics and Physics
- 5. Blaž Fortuna, B. Sc., Jožef Stefan International Postgraduate School, Ljubljana
- 6. Matej Gašperin, B. Sc., University of Nova Gorica
- 7. Dr. Dejan Gradišar, University of Ljubljana, Faculty of Electrical Engineering
- 8. Dr. Andrej Hrovat, Jožef Stefan International Postgraduate School, Ljubljana
- 9. **Dr. Peter Jeglič**, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Mathematics and Physics
- 10. Dr. Boštjan Kaluža, Jožef Stefan International Postgraduate School, Ljubljana
- 11. Dr. Martin Klanjšek, University of Ljubljana, Faculty of Mathematics and Physics
- 12. Dr. Boštjan Končar, University of Ljubljana, Faculty of Mathematics and Physics
- 13. Jurij Koruza, B. Sc., University of Ljubljana, Faculty of Natural Sciences and Technology
- 14. Dr. Petra Kralj, Jožef Stefan International Postgraduate School, Ljubljana
- 15. Dr. Marjan Kromar, University of Maribor, Faculty of Energy Technology
- 16. Dr. Matjaž Leskovar, University of Ljubljana, Faculty of Mathematics and Physics
- 17. Dr. Mitja Luštrek, Jožef Stefan International Postgraduate School, Ljubljana
- 18. Dr. Andrej Mihelič, University of Ljubljana, Faculty of Mathematics and Physics
- 19. Dr. Matija Milanič, University of Ljubljana, Faculty of Mathematics and Physics
- 20. Dr. Natan Osterman, University of Ljubljana, Faculty of Mathematics and Physics
- 21. Dr. Rok Pestotnik, University of Ljubljana, Faculty of Mathematics and Physics
- 22. Dr. Vid Podpečan, University of Ljubljana, Faculty of Mathematics and Physics
- 23. Vladimir Radulovič, University of Nova Gorica, School of Applied Sciences
- 24. Eva Ribežl, B. Sc., University of Ljubljana, Faculty of Mathematics and Physics
- 25. Dr. Andrej Prošek, University of Ljubljana, Faculty of Mathematics and Physics
- 26. Dr. Igor Sega, University of Ljubljana, Faculty of Mathematics and Physics
- 27. Dr. Andrej Studen, University of Ljubljana, Faculty of Mathematics and Physics
- 28. Tina Šfiligoj, B. Sc., University of Ljubljana, Faculty of Mathematics and Physics
- 29. **Dr. Miha Škarabot**, University of Ljubljana, Faculty of Chemistry and Chemical Technology and Faculty of Mathematics and Physics
- Dr. Primož Škraba, University of Ljubljana, Faculty of computer and information science
- 31. Tea Tušar, M. Sc., Jožef Stefan International Postgraduate School, Ljubljana
- 32. Dr. Mitja Uršič, University of Ljubljana, Faculty of Mathematics and Physics
- 33. Dr. Matjaž Vencelj, University of Ljubljana, Faculty of Mathematics and Physics
- 34. Dr. Vedrana Vidulin, Jožef Stefan International Postgraduate School, Ljubljana
- 35. Dr. Mojca Vilfan, University of Ljubljana, Faculty of Mathematics and Physics
- 36. Dr. Darko Vrečko, University of Nova Gorica, School of Environmental Sciences
- 37. **Dr. Andrej Zorko**, University of Ljubljana, Faculty of Natural Sciences and Technology and Faculty of Chemistry and Chemical Technology
- 38. Žerovnik Gašper, University of Maribor, Faculty of Energy Technology
- 39. Dr. Dušan Žigon, Jožef Stefan International Postgraduate School, Ljubljana

DELEGATIONS AND VISITORS

Members of the National Assembly of the Republic of Slovenia, 17 January 2013

Ms Alenka Bratušek, Prime Minister of the Republic of Slovenia 17 April 2013

Ms Sunita Williams, Astronaut, 20 May 2013

Delegation of Kimberly-Clark Corporation, 22 April 2013

Delegation of Filc, d. d., Škofja Loka, 17 June 2013

Prof. Hiroshi Ishiguro, Hiroshi Ishiguro Laboratories, ATR, Japan, 11 October 2013

Delegation of Yaskawe, Japan, 12 November 2013

Delegation of UNIDO-ICPE, 18 November 2013

Delegation of National Center for Scientific Research (Centre National de la Recherche Scientifique - CNRS), France, 18 November 2013 Ms Francesca Grassia, Deputy Director of European Research Area-East Ms Florence Noble, Deputy Scientific Director, Institute of Biological Sciences (INSB)



Sunita Williams and Prof. Jadran Lenarčič

ART EXHIBITIONS AT THE JSI

Riko Debenjak, 21 January-14 February Borut Peterlin, 18 February-14 March Srečo Dragan, Lujo vodopivec, Tugo Šušnik, 18 March-11 April Zvonko Čoh, 15 April-9 May Jože Slak-Đoka, 13 May-6 June Barbara Demšar, 10 June-4 July Ljubljana Fine Artists Society, 8 July-29 August Maša Gala, 2 September-26 September Adolf Mljač, 30 September-24 October Sašo Vrabič, 11 November-5 December

Gregor Pratneker, 9 December- 16 January 2014



Prof. Jadran Lenarčič, Director of the JSI, and Srečo Dragan at the opening of the exhibition

INSTITUTE COLLOQUIA

16 January: **Marko Bohanec** Jožef Stefan Institute *Qualitative multiparametric modeling and DEX method: Yesterday, today, and tomorrow*

30 January: **Gregor Anderluh** National Institute of Chemistry, Ljubljana *Biological nanopores*

20 February: **Sadamichi Maekawa** Tohoku University, Sendai, Japan *Spin-motive force as a new energy conversion mechanism*

6 March: **Antonio Šiber** Institute of Physics, Zagreb, Croatia **Some physics of viruses and the grand questions still unanswered**

19 March: **Peter Suhadolc** University of Trieste, Trieste, Italy *Achievements and challenges of modern seismology*

21 March: **Janez Bonča** University of Ljubljana and Jožef Stefan Institute **Nonequilibrium dynamics of correlated systems**

22 March: **Luka Snoj** Jožef Stefan Institute *Will we generate energy from water?*

28 March: Luiz A. DaSilva Trinity College, Dublin, Ireland Orchestrating virtual wireless networks from shared resource pools

3 April: **Cristian Micheletti** Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy *The knotted strands of life*

9 April: Luigi Colombo Texas Instruments Incorporated, Dallas, USA *Graphene and graphene device integration: A materials perspective*

24 April: **Boštjan Zalar** Jožef Stefan Institute *Liquid-crystalline elastomers: In search of morphing plastics*

8 May: Juergen Kurths

Potsdam Institute for Climate Impact Research and Humboldt University Berlin, Berlin, Germany, and University of Aberdeen, Aberdeen, Great Britain *Synchronization in dynamical systems and complex networks and its applications*

22 May: Maja Čemažar Institute of Oncology, Ljubljana Application of electroporation in medicine: Electrochemotherapy and electrogene therapy

5 June: **Hrvoje Buljan** University of Zagreb, Zagreb, Croatia *Ultracold atomic gases as quantum abacus beads*

28 August: **Milovan Šuvakov** Institute of Physics, Belgrade, Serbia *The Newtonian three-body problem: 13 new periodic solutions and topological classification*

13 September: **Grzegorz Wrochna** National Centre for Nuclear Research at Swierk, Otwock-Swierk, Poland *Nuclear power today and tomorrow*

17 September: **Yosef Nir** Weizmann Institute of Science, Rehovot, Israel *Flavor physics: past, present, future*

11 October: **Hiroshi Ishiguro** Osaka University, Osaka and Advanced Telecommunications Research Institute International, Kyoto, Japan **Robots, humans, and media**

27 November: **Miran Čeh** Jožef Stefan Institute *Scanning transmission electron microscopy: Applications in materials science*

4 December: **Slobodan Žumer** University of Ljubljana, Jožef Stefan Institute, and NAMASTE Center of Excellence *Topological soft matter*

11 December: **Saša Novak Krmpotič** Jožef Stefan Institute *Materials for bone replacement and regeneration*

FINANCING

REVENUES JSI (€) AND NUMBER OF PROJECTS

		Contribution		Contribution		No. of Projects
	2013	2013	2012	2012	Index 2013/2012	in 2013
National Agencies and Ministries	31,811,691	68.5 %	33,267,535	71.1 %	95.5	464
National Market	5,598,584	12.0 %	5,012,171	10.7 %	111.7	193
International Market	8,526,897	18.4 %	7,924,955	16.9 %	107.6	326
Other Revenues	526,217	1.1 %	585,646	1.3 %	95.5	
TOTAL	46,463,389	100.0 %	46,790,307	100.0 %	99.3	983



POSTGRADUATES FINANCED

1985-2013





Annual Report 2013

JSI UNDERGRADUATE SCHOLARSHIPS

1977-2013

Year]	FMF	FKKT	FKKT	NTF	FDV	FA	BF	FE and	Other	FG and	UNG	IPS	Total
			UNI LJ	UNI MB					FRI	UNI LJ	FERI			
1982	115	38	100						50	12				315
1983	10	1	5						9		1			26
1984	11	3	7					1	12		1			35
1985	18	4	6					1	19		1			49
1986	16	8	4						22	2				52
1987	20	8	4						23	2				57
1988	26	7	8					1	27	2				71
1989	26	6	10					1	19	3	1			66
1990	26	5	11					2	25		1			70
1991	23	2	9					2	24	2	1			63
1992	22	3	16					3	17	1				62
1993	21	1	15					3	13	1				54
1994	7	1	8					3	6					25
1995	2		9					3	5					19
1996	2		9					3	5					19
1997	2		12					1	4		1			20
1998	1		6					1	7		1			16
1999	2		7					4	7					20
2000	1		5					3	9					18
2001	3		13					3	10					29
2002	4		20					3	10					37
2003	3		18					2	12	1				36
2004	4		17					1	15	1	2	2		42
2005	3		12			1		2	19		2	1		40
2006	2		12			1		1	17		2	2		37
2007	3		14			1		2	18		2	1		41
2008	2	1	13	3		1		2	15		1	1		39
2009	2	1	17	4		1		5	16		1	2		49
2010	2		11	5	2	1	1	3	10		1	2	5	43
2011	2	1	11	5	4	1	1	4	7		1		6	43
2012	2		10	6	3	1		3	6				5	36
2013	3	2	3	2	1		1		2	2			6	22
TOTAL	386	92	422	25	10	8	3	63	460	29	20	11	22	1551
FMF FKKT (Uni-Lj) FKKT (Uni-Mb) NTF	Faculty of Faculty of Faculty of Faculty of	Mathematics and Chemistry and Ch Chemistry and Ch Natural Sciences	l Physics, Univ emical Techno emical Techno and Engineer	versity of Ljub ology, Universi ology, Universiti	ljana ty of Ljubljana ity of Maribor v of Ljubljana	L	FE FRI FG		Faculty of Elec Faculty of Con Faculty of Civ	ctrical Engine nputer and In il Engineering	ering, Univers formation Scie g, University o	sity of Ljublj ence, Univers f Maribor	ana sity of Ljublja	ina

FDV

FA

BF

Faculty of Pharmacy, Faculty of Mechanical Engineering, Faculty of Economics, Faculty of Medicine, University of Ljubljana

COMPLETED THESES

UNTIL 2013

Year	Ph. D. Theses	M. Sc. Theses	Total	Year	Ph. D. Theses	M. Sc. Theses	Total
1962	15	6	21	1988	12	26	38
1963	7		7	1989	15	33	48
1964	7	2	9	1990	16	41	57
1965	16		16	1991	22	47	69
1966	2		2	1992	19	42	61
1967		8	8	1993	28	36	64
1968	4	8	12	1994	27	37	64
1969	3	6	9	1995	34	22	56
1970	2	12	14	1996	38	25	63
1971	7	6	13	1997	29	23	52
1972	11	24	35	1998	21	20	41
1973	8	14	22	1999	33	29	62
1974	21	10	31	2000	36	27	63
1975	10	20	30	2001	31	28	59
1976	6	31	37	2002	29	19	48
1977	5	16	21	2003	41	19	60
1978	10	20	30	2004	31	20	51
1979	7	11	18	2005	22	7	29
1980	13	10	23	2006	22	2	24
1981	12	15	27	2007	26	7	33
1982	13	18	31	2008	29	5	34
1983	5	10	15	2009	30	7	37
1984	14	17	31	2010	33	5	38
1985	6	14	20	2011	31	2	33
1986	8	15	23	2012	47	4	51
1987	18	21	39	2013	56	7	63



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- S. G. Psakhie, Volia Isaevich Itin, D. A. Magajeva, O. G. Terehova, E. P. Najden, Olga Vasiljeva, Georgij Mihajlov Andrejevič, Urška Mikac, Boris Turk Contrast agent for T1 and/or T2 magnetic resonant scanning and method for preparing it
 - Patent No. RU2471502 (C1), Federal Service for Intellectual Property, 10.1.2013.
- Bojan Likar, Robert Posel, Andreas Kalagasidis, Tomaž Javornik, Gorazd Kandus, Janez Sterle, Urban Sedlar, Janez Bešter, Andrej Kos, Luka Mali Method for self organizing network operation Patent No. US8472334 (B2), US Patent Office, 25.6.2013.
- Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih Procedure for synthesis of threadlike tungsten oxide W5014 Patent No. US8496907 (B2), US Patent Office, 30.7.2013.
- Luca Gregoratti, Marco Peloi, Marija Kosec, Danjela Kuščer, Giuseppina Palma A material in the form of lithium fluoride powder containing colour centres, method for preparation and use thereof Patent No. US8535434 (B2), US Patent Office, 17.9.2013.
- Janez Pirš, Matej Bažec, Silvija Pirš, Bojaan Marin, Bernarda Urankar, Dušan Ponikvar

Variable contrast, wide viewing angle LCD light-switching filter Patent No. US8542334 (B2), US Patent Office, 24.9.2013.

- Bojan Likar, Robert Posel, Andreas Kalagasidis, Tomaž Javornik, Gorazd Kandus, Mihael Mohorčič, Aleš Švigelj, Janez Bešter, Andrej Kos, Miha Smolnikar Iterative localization techniques Patent No. US8565106 (B2), US Patent Office, 22.10.2013.
- Ida Istinič, Meti Buh Gašparič, Jerica Sabotič, Kristina Gruden, Jože Brzin, Jana Žel Use of macrocipines as pesticidal agents Patent No. SI23835 (A), Slovenian Intellectual Property Office of Russia, 28.2.2013.
- Matjaž Gams, Rok Piltaver, Erik Dovgan, Andrej Planina, Gašper Pintarič, Bogdan Pogorelc

Intelligent surveillance system and procedure for detection of unusual behaviour Patent No. SI23855 (A), Slovenian Intellectual Property Office, 28.2.2013.

 Borut Štrukelj, Samo Kreft, Damjan Janeš, Nina Kočevar Glavač, Eva Tavčar, Marko Slokar, Ante Zaloker, Viktor Grilc, Ivan Mirt, Željko Cerovečki Complex antioxidant extract from the bark of fir tree with cyclodextrins Patent No. SI23862 (A), Slovenian Intellectual Property Office, 29.3.2013. Borut Štrukelj, Samo Kreft, Damjan Janeš, Nina Kočevar Glavač, Eva Tavčar, Marko Slokar, Ante Zaloker
 Pefined liquid antioxidant avtract from the bark of fir tree and process for its

Refined liquid antioxidant extract from the bark of fir tree and process for its production

Patent No. SI23867 (A), Slovenian Intellectual Property Office, 29.3.2013.

- Silvan Bucik, Borut Baričevič, Borut Repič, Matjaž Vencelj A method of analog and digital signal processing of information contained in pulses, and a device for achieving the same. Patent No. SI23959 (A), Slovenian Intellectual Property Office, 28.6.2013.
- Andrej Kovič, Adolf Jesih, Aleš Mrzel The procedure for the synthesis of 4d and 5d (Nb, Mo Ta, W) nitrites of transition metals in the form of quasi-one-dimensional structures Patent No. SI23988 (A), Slovenian Intellectual Property Office, 30.8.2013.
- Kostja Makarovič, Janez Holc, Darko Belavič, Marko Hrovat, Marija Kosec Multilayer ceramic structures for non-contact dielectric heating of liquids Patent No. SI24008 (A), Slovenian Intellectual Property Office, 30.8.2013.
- Primož Titan, Jernej Iskra, Vladimir Meglič Chemical hybridization of hermaphrodite plant species with easily soluble derivatives of oxanilic acid Patent No. SI24033 (A), Slovenian Intellectual Property Office, 30.10.2013.
- 14. Gregor Černe, Mitja Bizjak, Bogdan Filipič, Tea Tušar, Erik Dovgan A system for offer selection and request formation in demand response and distributed production of electrical energy

Patent No. SI24057 (A), Slovenian Intellectual Property Office, 30.10.2013.
Marina Santo-Zarnik, Darko Belavič, Marjan Hodnik, Sandi Kocjan A pressure-sensor module with a ceramic cantilever sensing structure

- Patent No. SI24085 (A), Slovenian Intellectual Property Office, 29.11.2013. 16. Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov
- Composites materials based on ceramic phase and metal with functionalized surface as environmentally-friendly materials with antibacterial activity, a process for preparing and use thereof Patent No. SI24094 (A), Slovenian Intellectual Property Office, 31.12.2013.
- 17. Igor Kovač, Borut Lenart, Bojan Nemec, Marko Scortegagna, Leon Žlajpah Humanoid torso mechanism

Patent No. SI24099 (A), Slovenian Intellectual Property Office, 31.12.2013.

AWARDS AND APPOINTMENTS

AWARDS MADE TO JSI RESEARCHERS BY THE REPUBLIC OF SLOVENIA

Zois Award and Zois Certificate of Recognition

Janko Kos

Presented with the Zois Award for the highest scientific achievements in the field of proteolytic enzymes and their regulation

Nada Lavrač

Presented with the Zois Certificate of Recognition for her work in intelligent data analysis

Saša Novak Krmpotič

Presented with the Zois Certificate of Recognition in the field of materials

JSI AWARDS AND APPOINTMENTS

The Jožef Stefan Golden Emblem Prize

presented to the following for doctoral theses with high impact :

Lev Vidmar

Influence of phonons on physics of strongly correlated electron systems

Jernej Jorgačevski Fusion pore properties of cultured rat lactotrophs

Marko Sedlaček Influence of surface topography on tribological behavior of contact surfaces

SELECTED OTHER AWARDS TO JSI RESEARCHERS

Nemanja Aničić, Award of the Henkel Slovenia Foundation for B. Sc. Thesis, Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, »Application of the population balance model for the prediction of concentrated emulsion droplet size distribution«.

Leon Bedrač, Krka Awards for PhD Thesis, Novo mesto, Slovenia, 2013

Marko Bohanec, Best paper reward on International Conference 26th Bled eConference - eInnovation: Challenges and Impacts for Individuals, Organizations and Society

Sandra Drev, Aleksander Rečnik, Nina Daneu, "Twinning and inclusions in chrysoberyl from Pratinhas, Brazil", MC2013 Best poster award in Materials scince at the MC2013 Microscopy Conference, Regensburg, Germany, 25 – 30 August 2013

Sašo Džeroski, Nikola Simidjievski, Ljupčo Todorovski, Best ICT paper on 5th Jožef Stefan International Postgraduate School Students Conference

Jernej Fesel Kamenik, "Svečana listina" award for exceptional scientific and educational achievements, University of Ljubljana



The winners of Zois Award and Zois Certificates of Recognition: Prof. Nada Lavrač, Prof. Janko Kos and Asst. Prof. Saša Novak Krmpotič

Matjaž Gams, Hristijan Gjoreski, Simon Kozina, Mitja Luštrek, 1st place at the international activity-recognition competition, EvAAL 2013 (Evaluating AAL Systems through Competitive Benchmarking), Norrköping, Sweden, The AAL Open Association, RAReFall

Medeja Gec, Matic Krivec, Kristina Žagar, Luka Suhadolnik, Darja Jenko, Goran Dražić, Miran Čeh, "Comparison of TEM lamella preparation techniques on titania nanotube-arrays/metal Ti interface", MC2013 Best poster award in Instrumentation and Methods, at the MC2013 Microscopy Conference, Regensburg, Germany, 25 – 30 August 2013

Matjaž Gomilšek, Prešeren Award of the Faculty of Mathematics and Physics for Diploma thesis, University of Ljubljana, Ljubljana, Time irreversible billiards

Nadja Hvala, The article "Modelling, simulation and control of an industrial, semibatch, emulsion-polymerization reactor" in Computers and Chemical Engineering Journal has according to Elsevier more than 500 downloads. It has been identified as one of the most downloaded articles in this journal in the period from Sept. 2012 -Aug. 2013 and has received a certificate for this contribution.

Marja Jerič, Miran Čeh, "Molten salt synthesis of Nb-doped Sr3Ti2O7 platelet seeds", The best poster among young researchers in the research field Nanomaterials and Nanotechnology, 21st Conference on Materials and Technology, Portorož, Slovenia, 13 – 15 November 2013

Nina Kostevšek, Kristina Žužek Rožman, Sašo Šturm, Spomenka Kobe, "Hybrid FePt/Au Nanoparticles With a Combined Magneto-Photothermal Effect", The best presentation among young researchers in the research field Nanomaterials and Nanotechnology, 21st Conference on Materials and Technology, Portorož, Slovenia, 13 – 15 November 2013

Primož Koželj, Best paper award, Ljubljana, The European Integrated Center for the Development of New Metallic Alloys and Compounds, C-MAC days 2013, Ljubljana

Marjeta Kramar Fijavž, Best University Teacher Award at Department of Civil Engineering, University of Ljubljana, Faculty of Civil and Geodetic Engineering, awarded by the Student Council of the Faculty, Ljubljana, December 2013 Igor Križaj, Adrijana Leonardi, Dušan Kordiš, Award of the Slovenian Research Agency for an exceptional scientific achievement in 2012 in Slovenia in the field of Biochemistry and Molecular Biology (Conus consors snail venom proteomics unveils functions, pathways and novel families involved in its venomic system)

Zdravko Kutnjak, Mentor awards in 2013, the Society of Young Researchers Slovenia

Sebastjan Peljhan, Maks Samec Awards for PhD Thesis in the field of Chemistry, Ljubljana, Slovenia, 2013

Vid Podpečan, The outstanding scientific achievement: Environment Orange4WS for service-oriented data mining, Applicant: Public Research Agency of the Republic of Slovenia (SRA), the Scientific Council for Engineering

Aleksandra Rashkovska, Special prize for innovations for economy at the 6th International Transfer Conference and Innovation Day 2013, Brdo pri Kranju, Smart Thermo Therapy

Peter Rodič, Ingrid Milošev, Jernej Iskra, Barbara Kapun, 1st prize at the 6th International Conference for technology transfer together with Innovation Day of the Chamber of Commerce of Slovenia for innovation with largest market potential after the selection of local and foreign experts in the field of technology transfer and representatives of domestic and foreign venture capital, 2013

Luca Tubiana, Best PhD Thesis in Physics Award, Trieste, Italy, SISSA-ISAS.

Alenka Vesel, Award for the most cited article in the Journal Dyes and Pigments in years 2010 and 2011. Title of the article: "Colorimetric properties of reversible thermochromic printing inks"

Tea Zuliani, Radmila Milačič, Janez Ščančar, the Poster Prize at the «2013 Winter Conference on Plasma Spectrochemistry» taking place in Krakow, Poland, 10–15 February 2013, for her presentation entitled "Cr(VI) determination in soil solution by speciated isotope dilution ICP-MS"

In 2013 United Nations and UNESCO award Videolectures.Net portal for best educational product of the decade. The VideoLectures.Net was selected as the winner in the "e- Science & Technology" category



The winners of the Jožef Stefan Golden Emblem Prize: Dr. Lev Vidmar, Dr. Jernej Jorgačevski and Dr. Marko Sedlaček

REVIEW OF PUBLICATIONS

FOR 2013

Department	Original Articles*	Books	Patent Appl and	Theses
Department	original fit deles	DOORS	Grants	1110505
Department of Theoretical Physics (F-1)	95			4
Department of Low and Medium Energy Physics (F-2)	75		2	1
Department of Thin Films and Surfaces (F-3)	22			
Department of Surface Engineering and Optoelectronics (F-4)	59			
Department of Solid State Physics (F-5)	140		4	8
Department for Complex Matter (F-7)	50		2	4
Department of Reactor Physics (F-8)	34	4		2
Department of Experimental Particle Physics (F-9)	208			3
Department of Inorganic Chemistry and Technology (K-1)	38		2	2
Department of Physical and Organic Chemistry (K-3)	27		3	3
Electronic Ceramics Department (K-5)	51		4	2
Engineering Ceramics Department (K-6)	10			1
Department for Nanostructured Materials (K-7)	66	2	1	3
Department for Synthesis of Materials (K-8)	28			1
Department for Advanced Materials (K-9)	37		2	1
Department of Biochemistry, Molecular and Structural Biology (B-1)	35		2	2
Department of Molecular and Biomedical sciences (B-2)	16			1
Department of Biotechnology (B-3)	58	2	3	
Department of Environmental Sciences (0-2)	122			7
Department of Automation, Biocybernetics and Robotics (E-1)	46		2	3
Department of Systems and Control (E-2)	67		2	
Artificial Intelligence Laboratory (E-3)	43	1		
Laboratory for Open Systems and Networks (E-5)	15			
Department of Communication Systems (E-6)	47		3	2
Computer Systems Department (E-7)	28			1
Department of Knowledge Technologies (E-8)	64			5
Department of Intelligent Systems (E-9)	64	1	4	5
Department of Reactor Engineering (R-4)	56	1		1
Reactor Infrastructure Centre (RIC)	21	3		
Networking Infrastructure Centre (NIC)	1			
Science Information Centre (SIC)	1			
Energy Efficiency Centre (EEC)	21			
Milan Čopič Nuclear Training Centre (ICJT)	4			
Radiation Protection Unit (SVPIS)	1	1		
Centre for Technology Transfer and Innovation (CTT)	2			1
Jožef Stefan Institute	1533	13	32	63

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

KNOWLEDGE TRANSFER

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

R & D PROJECT PARTNERS

- 1. Abak.net, d.o.o., Murska Sobota
- 2. Acies Bio, d.o.o., Ljubljana
- 3. Adria Mobil, d.o.o. Novo mesto
- 4. Akripol, d.o.o., Trebnje
- 5. Amebis, d.o.o., Kamnik
- 6. Ames, d.o.o., Brezovica pri Ljubljani
- 7. ARAO-Slovenian Agency for Radioactive Waste Management,, Ljubljana
- 8. Arctur, d.o.o., Nova Gorica
- 9. B2, d.o.o., Ljubljana
- 10. Balder, d.o.o., Ljubljana
- 11. Beyond Devices, d.o.o., Brezovica pri Ljubljani
- 12. BIA Separations, d.o.o., Ajdovščina
- 13. CDT skupina, d.o.o., Kropa
- 14. Central Technological Library at the University of Ljubljana, Ljubljana
- 15. Chemicals Office of the Republic of Slovenia, Ljubljana
- 16. Cosylab, d.d., Ljubljana
- 17. Creatim Ržišnik Perc, d.o.o., Šenčur
- 18. Development Centre RC eNeM, d.o.o., Ljubljana
- 19. Domel, d.o.o., Železniki
- 20. Ecological Engineering Institute, d.o.o., Maribor
- 21. Ekliptik, d.o.o., Ljubljana
- 22. Elgoline, d.o.o., Cerknica
- 23. Ema, d.o.o., Celje
- 24. Entia, d.o.o., Ljubljana
- 25. Gama System, d.o.o., Ljubljana
- 26. Gen energija, d.o.o., Krško
- 27. Gorenje, d.d., Velenje
- 28. Inea, d.o.o., Ljubljana
- 29. Informa Echo, d.o.o., Ljubljana
- 30. Institute of Microbial Sciences and Technologies, d.o.o., Domžale
- 31. Intec Tiv, d.o.o., Kranj
- 32. Intech Les, d.o.o., Rakek
- 33. JP CČN Domžale-Kamnik, d.o.o., Domžale
- 34. JP Vodovod-Kanalizacija, d.o.o, Ljubljana
- 35. Keko Oprema, d.o.o., Žužemberk
- 36. Knauf Insulation, d.o.o., Škofja Loka

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.

- 37. Kolektor Group, d.o.o., Idrija
- 38. Kolektor KFH, d.o.o., Idrija
- 39. Kolektor Sikom, d.o.o., Idrija
- 40. Kovinos, d.o.o., Horjul
- 41. Krško Nuclear Power Plant, Krško
- 42. Labena, d.o.o., Ljubljana
- 43. Lek, d.d., Ljubljana
- 44. Lotrič Metrology, d.o.o., Selca
- 45. Magneti Ljubljana, d.d., Ljubljana
- 46. MEIS storitve za okolje, d.o.o., Šmarje Sap
- 47. Melamin kemična tovarna d.d., Kočevje
- 48. Metrology Institute of the Republic of Slovenia, Celje
- 49. Milan Vidmar Electric Power Research Institute, Ljubljana
- 50. Ministry of Education, Science and Sport of the Republic of Slovenia, Ljubljana
- Ministry of Infrastructure and Spatial Planning of the Republic of Slovenia, Ljubljana
- 52. Ministry of Defence of the Republic of Slovenia, Ljubljana
- 53. Optacore, d.o.o., Ljubljana
- 54. Research Centre Energy, d.o.o., Velenje
- 55. Result, d.o.o., Ljubljana
- 56. Robotina, d.o.o., Kozina
- 57. Slovenian Environment Agency, Ljubljana
- 58. Solvera Lynx, d.d., Ljubljana
- 59. Stelem, d.o.o. Žužemberk,
- 60. Stirolab, d.o.o., Sežana
- 61. Špica International, d.o.o., Ljubljana
- 62. Štore Steel, d.o.o., Štore
- 63. Technology Park Ljubljana, d.o.o., Ljubljana
- 64. UCS, d.o.o., Vrhnika
- 65. Unior, d.d., Zreče
- 66. Vacutech, d.o.o., Ljubljana
- 67. Varsi, d.o.o., Ljubljana
- 68. Velenje Coal Mine, d.d., Velenje
- 69. Xenya, d.o.o., Ljubljana
- 70. Xlab, d.o.o., Ljubljana



INSTITUTE IN NUMBERS

2012-2013

COMPARISON OF REVENUES (€M)

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



EMPLOYEES (FTE)



REVENUES FROM PUBLIC SERVICES (€M)



NUMBER OF PUBLICATIONS IN THE WEB OF SCIENCE



NUMBER OF CITATIONS IN THE WEB OF SCIENCE



RESEARCH DEPARTMENTS

DEPARTMENT OF THEORETICAL PHYSICS F-1

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

Meson scattering and electroproduction in the D13, D33 and D15 partial waves are calculated in a coupledchannel approach incorporating quasi-bound quark-model states. In contrast to our previous results in the P11, P33 and S11 partial waves, the meson and photon couplings turn out to be underestimated, but otherwise our results exhibit a consistent behaviour in all channels.

The unambiguous evidence for the interesting state X(3872) was found using an ab-initio lattice QCD simulation for the first time. This charmonium-like state is particularly interesting since it is most likely a mesonic molecule. The exciting state Zc(3900), which was experimentally discovered in the spring of 2013 and is composed of two quarks and two anti-quarks, was simulated on the lattice for the first time. We studied the meson decay widths Head: using the extended method we proposed last year and demonstrated how it works in practice by determining the Prof. Svjetlana Fajfer K*(892), D0*(2400) and D1(2430) strong decay widths.

aces o

In the past year we implemented a new state-of-the-art method called stochastic distillation, which allowed us to calculate correlation functions on a 3fm lattice. We used this method to study the controversial meson Ds(2317), where we confirmed experimentally observed properties and settled a longstanding issue between theory and experiment.

We performed an analysis of Higgs portal models of dark matter (DM), where DM is light enough to contribute to invisible Higgs decays. Using effective field theory we showed that DM can be a thermal relic only if there

are additional light particles present with masses below a few 100 GeV. We also gave three concrete examples of viable Higgs portal models of light DM. We systematically investigated the implications of the leading dimension five

operators on Higgs phenomenology in the presence of dynamical vector-like quarks. After taking into account the constraints from precision electroweak and flavour observables we showed that contrary to the renormalizable models, significant modifications of the Higgs' properties are still possible. We reconsidered the recent observation by the D0 experiment of a sizable like-sign dimuon charge asymmetry, highlighting that it could be affected by CP-violating contributions not only in Bd- and Bs-meson mixings, but also in semi-leptonic decays of b and c quarks. We also showed that such effects would be clear indications of new physics. We showed that warped extradimensional models that explain the quark spectrum can naturally give rise to contributions of the size required to explain the recent LHCb result for a CP violation in D meson decays. We also explained important subtleties in the calculations of certain one-loop processes within warped extra-dimensional models. We furthermore discussed the interpretation of this result within the framework of partial compositeness in four dimensions.

An explanation for the too large measured branching fraction of decays B -> D tau nu in B -> D* tau nu has still not been provided and the result of the BaBar collaboration is still valid. We have studied a scenario with the addition of a single scalar particle that couples to quarks and leptons. We have endowed this leptoquark with the quantum number (3,2,7/6) and a minimal set of flavour coupling that suffices to explain the B -> D(*) tau nu anomaly and is consistent with constraints from other processes. These are decay Z -> b anti-b, lepton flavour violating decays (e.g., mu -> e gamma), and magnetic and electric dipole moments. In the framework of a Grand

We found the first evidence for the interesting state X(3872) using ab-initio lattice QCD simulations. We performed an exhaustive theoretical analysis of the Higgs' portal models of cosmological dark matter.



Figure 1: Constraints on the couplings of leptoquark to $(b\tau)$ and to $(c\mu)$ coming from the 1σ region of $Br(B \rightarrow D(*) tau nu)$ (thin hyperbolic region), and from 90% CL upper bounds on $\mu \rightarrow e\gamma$, $\tau \rightarrow \mu\gamma$ and $\tau \rightarrow e\gamma$.

Unified Theory we have predicted correlations between the various decay channels of the proton, as well as rare decays of the t-quark and D meson.

We solved the equation for perturbations of a scalar field in AdS with no back-reaction. Through the holographic prescription we showed in this way the existence of a massless pole in the propagator of the boundary theory in the case of vev deformation, in contrast with an earlier claim in the literature.

In the framework of the minimal left-right symmetric model, an original connection between the Dirac and Majorana masses was established. This link removes the indeterminacy of the Dirac mass of neutrinos and allows for a direct correlation between potential measurements of heavy neutrinos and a number of other experiments. We investigated the signals of the Dirac mass at the LHC collider, neutrino-less double beta decay and the electric dipole moment of the electron.

We investigated the problem of positive and negative energies occurring in the quantum field theories in ultrahyperbolic spaces, and in the theories with higher derivatives. We found that under certain conditions such theories can be stable, for instance, if the interaction potential is bound from below and from above.

Some outstanding publications in the past year

- 1. Prelovšek, S., Leskovec, L.: Evidence for X(3872) from DD* scattering on the lattice, Phys.Rev.Lett. 111 (2013)
- Fajfer, S., Greljo, A., Kamenik, J., Mustać, I.: Light Higgs and vector-like quarks without prejudice. The Journal of high energy physics, ISSN 1126-6708, 2013, vol. 2013, no. 7, 155 (2013)

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.

In the theory of non-equilibrium properties of correlated electrons we continued our research of various prototype models with the emphasis on a numerical simulation of undoped and weakly doped Mott insulators. We have investigated the ultra-fast optical response of the one-dimensional Hubbard model that was exposed to two consecutive laser pulses. Using the time-dependent Lanczos method we have discovered that through the selection of the pulse sequence one can excite and de-excite excitons in these systems. In fermion and boson systems

We have investigated the phenomenon of the ultrafast recombination of photo-excited charged particles in undoped insulating cuprates and developed a theory that is based on multiple magnon emission.



Figure 2: Graph of emotional communications in online chats (the red and black colours indicate messages carrying positive and negative emotions, respectively, while the blue colour shows emotionally neutral messages.)

we investigated the basic properties of the out-of-equilibrium dynamics in near-integrable models, also in relation to experiments on ultra-cold atoms on optical lattices. We studied the ultra-fast relaxation and recombination of charged particles that are photo-induced in undoped insulating cuprates and proposed a theory that is based on the emission of multiple magnons and supported it by numerical calculations within the single-band effective model, reaching a good agreement with the measured recombination times. We have introduced the reduced density matrix method to problems of thermal properties of the isolated out-of-equilibrium correlated systems and discovered a deviation from the standard level statistics in the presence of an external field.

On the subject of the equilibrium properties of correlated electrons we have calculated several thermodynamic properties of the Hubbard model on the anisotropic triangular lattice that describes well the organic superconductors and observed numerically the metal-insulator transition. We have investigated the transport in the doped Mott insulators and discovered well-defined, quasi-particle-like excitations well beyond the Fermi liquid regime. Using the dynamical mean-field theory we have established the ferromagnetic phases of the Kondo-lattice and investigated the topological transitions between them. We have investigated the optical response of Fermi liquids. We published a review article on the influence of Hund's rule coupling in multi-orbital metals. Within a model of the disordered Heisenberg spin chain we explained the anomalously broad distribution of the NMR relaxation times in the mixed system BaCuSiGeO. In relation to the new measurements we have investigated the heat transport for a model of weakly coupled antiferromagnetic spin chains. In collaboration with the calorimetry group at the JSI we have modelled the ferroelectric barium titanite and calculated its phase diagram, the specific heat and the electro-calorical effect.

Within the theory of nanoscale systems we studied the coherent manipulation of the electronic spin in the quantum dot using the time-dependent driving of the harmonic potential and the spin-orbit coupling. We have calculated the spin-Seebeck coefficient for the two-channel Kondo model in the magnetic field and observed the thermal transition between the Fermi-liquid and the non-Fermi-liquid regimes. We have analysed the thermal entanglement in a system of three-spins in the triagonal geometry and have shown that the external electric field can induce a maximally entangled state. Using the density functional theory we have investigated the time dependence of the electronic transport through a quantum dot in the Coulomb blockade regime.

In the research on the statistical physics of complex systems and networks we analysed the empirical data from the world wide web and theoretically modelled it. We also simulated nano-systems using mathematical graphs of the nano-network. Within the CYBEREMOTIONS project we investigated the dynamics of the emotional interactions on the web. Theoretical models were devised for certain web-portals. We introduced nano-networks as a concept to determine the complexity at the nano-scale.

Some outstanding publications in the past year

- Deng, X., Mravlje, J., Žitko, R., Ferrero, M., Kotliar, G., Georges, A.: How bad metals turn good : how bad metals 1. turn good. Physical review letters, ISSN 0031-9007, 2013, vol. 110, no. 8, 086401
- 2. Lenarčič, Z., Prelovšek, P.: Ultrafast charge recombination in a photoexcited Mott-Hubbard insulator. Physical review letters, ISSN 0031-9007, 2013, vol. 111, iss. 1, 016401

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

We worked on several problems in the electrostatics of macromolecular solutions. Within the linearized Debye-Hückel approximation, we analysed the effect of the patchiness of charged macroions on the interactions

between them, deriving the conditions for this interaction to be dominant. Also discussed was the interaction between an anisotropic dielectric semiinfinite slab and a moving charge on top of it. We reviewed the recent advances in the field of Coulomb fluids. We showed to what extent they are able to capture effects known to elude the mean-field level of description. We studied the dielectric spectra of DNA in Mg ionic solutions. Various differences are observed when compared to the previously obtained dielectric

spectra in monovalent salt solutions and an effort has been made to explain these novel features. Using molecular dynamics simulations, we investigated the properties of biological membranes, focusing on the hydration repulsion between them.

We introduced a model of the helix-coil transition that allows for a straightforward generalization of the effects of solvent structure. In an extensive computational study, we explored the statics and the dynamics of long flexible linear polymers that spontaneously knot and unknot. Also investigated theoretically was the structure of nematic polymers, where we discussed a novel feature in terms of a differential tensorial constraint, which is expected to be important in a macroscopic description of, e.g., DNA ordering in a confined space. With our studies of optical properties of ferrofluids prepared by dispersing ferromagnetic cobalt nanoparticles in cyclohexane, we provided experimental verification of the flexible-chain model for nanoparticles in ferrofluids. We explored the ways of integrating topics on the physics of liquid crystals into undergraduate curricula.

We studied colloidal and nanoparticle ordering in polymer layers. Hard-core colloids form characteristic patterns with a well-defined length scale that can be externally controlled. Our theoretical results suggest several possible applications in miniature sensors, energy production and storage, as well as surface and particle characterization. We analysed the elastic interaction between model 2D colloidal particles and we showed that the non-pairwise aspect of the repulsion between them increases as the particles become more incompressible.

We explored a model of epithelial tissues based on the surface energy of cells, finding that the periodic equilibrium states of the epithelium can be either flat or corrugated. We reviewed the mechanical models of ventral furrow formation in a Drosophila embryo. Also investigated was the composite contact of two-component lipid membranes, which includes inverted micelles. Our determination of the positioning of integrin 1 and caveolin-1 on the membrane of adhered spreading cells showed that the presence of one of them spatially excludes the occurrence of the other. Recent experimental results on the aggregation of red blood cells and the corresponding beyonds, J. Chem. Phys. 139, 150901 (2013).

We have studied the optical properties of ferrofluids and have experimentally verified the flexible chain model, i.e., that nanoparticles in colloid suspensions form flexible chains.



Figure 3: Cover of the Journal of Chemical Physics highlighting our review paper on electrostatic interactions A. Naji, M. Kanduč, J. Forsman, and R. Podgornik, »Perspective: Coulomb fluids weak coupling, strong coupling, in between and

theoretical analyses of the depletion mechanism and of the influence of the cell shape on the adhesion strength were reviewed. The partitioning of fatty acids into phospholipid membranes was studied on giant unilamellar vesicles, utilizing phase-contrast microscopy, and the observed, enhanced partitioning under conditions of increased membrane strain was interpreted on the basis of a tension-dependent intercalation of oleic acid into the membrane. Finally, we analysed some pertinent questions of physical virology, dealing mostly with charge distribution and the effect of electrostatic interactions on proteinaceous viral shells.

Some outstanding publications in the past year

- 1. Šiber, A., Ziherl, P.: Many-body contact repulsion of deformable disks. *Physical review letters*, ISSN 0031-9007, 2013, vol. 110, no. 21, 214301
- 2. Naji, A., Kanduč, M., Forsman, J., Podgornik, R.: Perspective: Coulomb fluids weak coupling, strong coupling, in between and beyond. *The Journal of chemical physics*, ISSN 0021-9606, 2013, vol. 139, no. 15, 150901

Organization of conferences, congresses and meetings

- 1. Probing the Standard Model and New Physics at Low and High Energies, Portorož, 14.–18. 4. 2013
- 2. Physics of Complex Colloids, Ljubljana, 14.-18. 5. 2013
- 3. Selected Challenges in Particle Phenomelogy, Belica, 18.-20. 9. 2013
- 4. 8th Christmas Biophysics Workshop, Dobrna, 16.-17. 12. 2013
- 5. Non-equilibrium dynamics of Correlated Electron Systems, Krvavec, 18.-20. 12. 2013

Awards and appointments

- 1. Jernej Fesel Kamenik: "Svečana listina" award for exceptional scientific and educational achievements, University of Ljubljana
- 2. Luca Tubiana: Best Ph.D. Thesis in Physics Award, Trieste, Italy, SISSA-ISAS
- 3. Lev Vidmar: The Jožef Stefan Golden Emblem Prize for doctoral thesis, Jožef Stefan Institute, Ljubljana

INTERNATIONAL PROJECTS

- 1. 7FP Cyberemotions; Collective Emotions in Cyberspace European Commission Prof. Bosiljka Tadić
- 7FP LOTHERM; Low Dimensional Quantum Magnets for Thermal Management European Commission Prof. Peter Prelovšek
- 7FP COMPLOIDS, Physics of Complex Colloids: Equilibrium and Driven European Commission
- Prof. Primož Ziherl 4. COST TD1210; Analysing the Dynamics of Information and Knowledge Landscapes COST Office
- Prof. Bosiljka Tadić
- Theoretical Studies of Dynamical Properties in Correlated Electron Systems Coupled to External Degrees of Freedom Slovenian Research Agency
- Prof. Janez Bonča
- 6. Flavor Violation at the Large Hadron Collider
- Slovenian Research Agency Asst. Prof. Jernei Fesel Kamenik
- Aspects of the AdS-CFT Correspondence in Particle Physics and Cosmology Slovenian Research Agency Prof. Borut Baic
- Relaxation Dynamics of Correlated Electron Systems Slovenian Research Agency Prof. Janez Bonča

VISITORS FROM ABROAD

- 1. Dr. Christoph Bobet, Technische Universität, München, Germany, 9.-11. 1. 2013
- Dr. Robin Steinigeweg, Institut f
 ür theoretische Physik, Technische Universit
 ät Braunschweig, Braunschweig, Germany, 22.–27. 1., 26.-30. 11. 2013
- 3. Prof. Marcin Mierzejewski, University of Katowice, Poland, 6.-16. 2. 2013
- Prof. David Sherrington, University of Oxford, Oxford, Great Britain, 13. -14. 2. 2013
 Prof. Adrian Lugo, Departamento de Fisica and IFLP-CONICET, Facultad de Ciencias
- Exactas, Universidad Nacional de La Plata, La Plata, Argentina, 14. 2.-14. 3. 2014

RESEARCH PROGRAMS

- 1. 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. Rudolf Podgornik

R&D GRANTS AND CONTRACTS

- 1. Theoretical Aspects and Empirical Analysis of Labour Market Impact of Flexicurity Dr. Jernej Mravlje
- 2. Integrability and Ergodic Theory of Non-equilibrium Quantum Many-body Systems Dr. Jernej Mravlje
- 3. Non-equilibrium Dynamics of Interacting Electron Systems Prof. Peter Prelovšek
- . Synergies between precision measurements and LHC discoveries Asst. Prof. Jernej Fesel Kamenik
- Investigation of Strongly Interacting Electron Systems by a Computational Study of a Model for Organic Superconductors Dr. Jure Kokali
- 6. Dr. Pieralberto Marchetti, University of Padova, Padova, Italy, 20.-23. 2. 2013
- 7. Prof. Sadamichi Maekawa, Dr. Kenji Tsutsui, Prof. Takami Tohyama, Dr. Hantao Lu,
- 8. Dr. Wataru Koshibae, Koudai Sugimoto, Kazuya Shinjo, Shigetoshi Sota, Yukawa
- Institute of Theoretical Physics, Kyoto University, Kyoto, Japan, 19.–21.2. 2013
 Dr. Krešimir Kumerički, Prirodnoslovno matematički fakultet, Sveučilište u Zagrebu, Zagreb. Croatia. 21, 2. 2013
- 10. Prof. Jan O. Eeg, Physics Department, Oslo University, Oslo, Norway, 25. 2.-1. 3. 2013

- 11. Dr. Marco Berrita, University of Lancaster, Lancaster, Great Britain, 28. 2.-28. 3., 25.11.-8.12.2013
- 12. Dr. Marco Budinich, ICTP and University of Trieste, Trieste, Italy, 18.-19. 3. 2013
- 13. Dr. Valentina Verduci, University of Graz, Graz, Austria, 20.-21. 3. 2013
- 14. Prof. Christian Wagner, Experimentalphysik Universität des Saarlandes, Saarbrücken, Germany, 20.-22. 3. 2013
- 15. Prof. Günther Meissner, Universität des Saarlandes, Saarbrücken and Technische Universität München, Germany, 25.-27.3.2013
- 16. Dr. Joachim Kopp, Max Planck Institute Heidelberg, Germany, 28.-29. 3. 2013 Prof. Frank Marsiglio, Department of Physics, University of Alberta and Physics 17.
- Division, School of Science and Technology, University of Camerino, Italy, 2.-3. 4. 2013 18. Dr. Benoit Schmauch, University of Saclay, Paris, France, 21.-25. 4. 2013
- 19. Denis Parganlija, Vienna University of Technology, Vienna, Austria, 24.-26. 4. 2013
- 20. Prof. Oleg Shushkov, University of South Wales, Sydney, Australia, 8.-13. 6. 2013
- 21. Prof. Rodolfo Jalabert, l'Institut de Physique et Chimie des Matériaux de Strasbourg and IPCMS,
- Département Magnétisme des Objets NanoStructurés, Strasbourgu, France, 1.-5. 7. 2013 22. Prof. Ilja Doršner, Univerza v Sarajevu, Institut za naravoslovje in matematiko,
- Sarajevo, BOSNIA, 6. 7.-18. 8., 13.-16. 10., 27.-30. 11., 15.-21. 12. 2013 23. Dr. Luca Di Luzio, Institut für Theoretische Teilchenphysik, Karlsruhe Institute of
- Technology (KIT), Karlsruhe, Germany, 31. 7.-4. 8. 2013 24. Prof. Tomonari Dotera, Kinki University, Osaka, Japan, 26.–31. 8. 2013
- 25. Dr. Berin Belma Sirvanli, Gazi University, Arts and Sciences Faculty, Department of Di-Derm John Julia, dazi Oniverski, files and ocerces race Physics, Ankara, Turkey, 2. 9.–30. 11. 2013
 Michael Park, Rutgers University, New Jersey, USA, 3.–6. 9. 2013
- 27. Dr. Dilip Ghosh, IACS, Kolkata, India, 12. 9. 2013

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- 17. Prof. Anton Ramšak*
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- 21. Dr. Milovan Šuvakov, left 01.03.13
- 22. Prof. Bosiljka Tadić
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26. Dr. Rok Žitko

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28. Dr. Jure Drobnak

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ORIGINAL ARTICLE

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- Borut Bajc, Adrián Lugo, "On the matching method and the Goldstone theorem in holography", J. high energy phys., vol. 2013, issue 7, pp. 56-1-56-16, 2013.
- 3. Christophe Berthod, Jernej Mravlje, Xiaoyu Deng, Rok Žitko, Dirk van der Marel, Antoine Georges, "Non-Drude universal scaling laws for the optical response of local Fermi liquids", Phys. rev. B, Condens. matter mater. phys., vol. 87, no. 11, pp. 115109-1-115109-15, 2013.

- 28. Prof. Josef Nir, Weizmann Institute, Rehovot, Israel, 15.-18. 9. 2013
- 29. Dr. Pablo Vazquez-Monteo, Departamento de Matemáticas Aplicadas y Sistemas,
- Universidad Autónoma Metropolitana-Cuajimalpa, Mexico, 22.-28. 9. 2013
- 30. Prof. Ross McKenzie, University of Queensland, Brisbane, Australia, 27. 9.-13. 10. 2013
- 31. Dr. Stephane Lavignac, Saclay University, Paris, France, 29. 9.-4. 10. 2013
- Sahib Babaee Tooski, Division of Theory of Solid State Physics, Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland, 2.-24. 10. 2013
- 33. Dr. Giannis Georgoiu, Technische Universität Wien, Vienna, Austria, 6.-12. 10. 2013
- 34. Prof. Kaladi Babu, Oklahoma State University, Stillwater, USA, 7.-8. 10. 2013
- 35. Prof. Qaisar Shafi, Bartol Research Institute, University of Delaware, Delaware, USA, 15. 10. 2013
- 36. Dr. Takehiro Jimbo, Tohoku University, Sendai, Japan, 20. 10.-20. 11. 2013
- Dr. Osor Slaven Barišić, Institut za fiziku, Zagreb, Croatia, 23.-24. 10. 2013
- 38. Prof. Masayuki Imai, Ochanomizu University, Tokyo, Japan, 13.-17. 11. 2013
- 39. Dr. Gabrijela Zaharijas, ICTP, Trieste, Italy, 14. 11. 2013
- 40. Dr. Markus Aichhorn, Technische Universität, Graz, Austria, 14.–16. 11. 2013
- 41. Antione Gerardine, Laboratoire de Physique Theorique d'Orsay, Orsay, France, 20.-22. 11. 2013
- 42. Prof. J. H. Jefferson, University of Oxford and QinetiQ, Great Malvern, Great Britain, 24. 11.-1. 12. 2013
- 43. Dr. Matteo Rauzi, European Molecular Biology Laboratory, Heidelberg, Germany, 25.-26.11.2013
- 44. Prof. Xenophon Zotos, University of Crete, Heraklion, Greece, 27.-30. 11. 2013
- 29. Dr. Ana Hočevar Brezavšček, left 02.07.13
- 30. Dr. Julio Julio, left 01.10.13
- 31. Dr. Matej Kanduč
- 32. Dr. Anže Lošdorfer Božič, left 01.11.13
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- 42. Dr. Tilen Huljev Čadež, left 01.06.13
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- 44. Jan Kogoj, B. Sc.
- 45. Matej Krajnc, B. Sc
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- 50. Ivan Nišandžić, B. Šc.
- 51. Žiga Osolin, B. Sc.
- 52. Vasja Susič, B. Sc.
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53. Nevenka Hauschild

Note: * part-time JSI member

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4. A. Bharucha et al. (44 authors), "Implications of LHCb measurements and future prospects", Eur. Phys. j. C, vol. 73, no. 4, pp. 2373-1-2373-92.2013 5. Oliver Bodensiek, Rok Žitko, Matthias Vojta, Mark Jarrel, Thomas

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MENTORING

- 1. Tilen Čadež, *Quantum entanglement in systems of strongly interacting electrons:* doctoral dissertation, Ljubljana, 2013 (mentor Anton Ramšak).
- 2. Jacek Herbrych, *Finite-temperature dynamics of quantum spin chains:* doctoral dissertation, Ljubljana, 2013 (mentor Peter Prelovšek).
- Anže Lošdorfer Božič, Interactions & geometry of self-assembly in viruslike particles: doctoral dissertation, Ljubljana, 2013 (mentor Rudolf Podgornik).
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- 5. Jerneja Pavlin, Liquid crystals as a means of introducing modern topics into teaching of physics: teaching module Liquid crystals for the highschool and university level: doctoral dissertation, Maribor, 2013 (mentor Nataša Vaupotič; co-mentor Mojca Čepič).
- Šaša Ziherl, Anisotropy of wood in the microwave region: doctoral dissertation, Maribor, 2013 (mentor Mojca Čepič; co-mentor Jurij Bajc).
- 7. Matej Krajnc, *Mechanical model of simple epithelian tissue*: master's thesis, Ljubljana, 2013 (mentor Primož Ziherl).
- Maruša Vitek, Change of form of phospolipid vesicles due to lipopolisacharid inclusion: master's thesis, Ljubljana, 2013 (mentor Saša Svetina; co-mentor Mojca Mally).

DEPARTMENT OF LOW AND MEDIUM ENERGY PHYSICS

The Department of Low and Medium Energy Physics is active in research in the field of atomic physics (low-energy physics) and nuclear physics (medium-energy physics). The acquired knowledge is applied for monitoring the ionizing radiation in the environment, as well as for interdisciplinary research with particle and photon beams. The Tandem Ion Accelerator at the department is one of the largest research facilities in the country. The department invested considerable efforts in the development of its own research instrumentation to enable a two-direction experimental research process: researchers from the department are performing research on large accelerator facilities abroad, and researchers from the European research area are accessing the instrumentation at the JSI ion accelerator in the frame of Transnational Access Program within the EU's 7FP.

F-2



Within the A1 Collaboration of the MAMI facility (Mainz, Germany) we have completed the first set of measurements on the elastic scattering of electrons on protons, in which the initial-state radiation (ISR) method is used to access the range of momentum transfers otherwise unreachable in a standard spectrometer configuration. The Head: main goal of the experiment is a determination of the elastic (electric and magnetic) form factors of the proton at Asst. Prof. Primož Pelicon momentum transfers below approximately 0.01 GeV2, thereby opening a way to the determination of the mean value of the proton radius, where the discrepancy between the values extracted from electron scattering and those determined in Lamb-shift measurements in muonic atoms remains unresolved. We have also continued to perform test measurements to search for dark photons, i.e., the hypothetical particle that couples ordinary and dark matter; we have developed several versions of target cells and tested them in beam environments in order to find the optimal model to be used in production measurements. We have finished the data-acquisition period for the virtual Compton scattering by measuring the only remaining kinematic setting with 0.5 GeV2. At present we are in possession of all three planned data sets at momentum transfers of 0.1, 0.2 and 0.5 GeV2 that will enable us to determine the generalized polarizabilities of the proton. The preliminary results of the analysis at 0.1 GeV2 are already available. The analysis of the data acquired in the recoil-polarization experiment (measurement of proton recoil polarization in neutral-pion electroproduction off protons in the region of the Roper resonance) is still on going.

In the Thomas Jefferson National Accelerator Facility (Jefferson Lab) we collaborated during the preparations for the real Compton scattering experiment at high momentum transfers, implying also large values of all the Mandelstam variables s, t and u. The main goal of the experiment is to measure the unpolarized cross-sections as functions of s and t to an accuracy of better than 10%. With such high-quality data we would be able to determine the actual power law that governs the scaling of cross-sections and thereby confirm or exclude the three proposed competing mechanisms of high-momentum scaling (perturbative QCD, approach based on generalized parton distributions and soft collinear effective theory).

In 2013 we studied electron screening in the nuclear reactions $58Ni(p,\gamma)59Cu, 60Ni(p,\gamma)61Cu, 50V(p,n)50Cr, 51V(p,\gamma)52Cr, 55Mn(p,\gamma)56Fe$ 55Mn(p,n)55Fe, 113Cd(p,n)113In, 115In(p,n)115Sn and 27Al(p,y)28Si. For these reactions we compared reaction cross-sections in metallic and insulating targets. Most insulating targets consisted of metallic oxides, only in the case of aluminium we additionally used a nitride target. In none of the above reactions did we observe any difference in the reaction rates between metallic and insulating targets. This contradicts the published results of a group from Bochum, Germany, which reported significant differences from 134302). measurements using two targets.



Figure 1: Widths of Ko. emission lines as a function of incoming photon energy for the 1st (lighter symbols) and 2nd (darker symbols) σ * resonances together with the dispersions and the widths for CH₂Cl₂ generated by the fit (black lines). (R. Bohinc et al. J. Chem. Phys. 139,

Within the Centre of Competency in Biomedical Engineering and its TOF-PET subproject, the final stages of development were performed and a provisional patent application filed to protect one of the key results for commercial exploitation. Furthermore, two different concepts for an angular-sensitive gamma camera were developed and successfully tested. Within the research on the analysis of signals from photon and particle detectors, a new approach for solid-state detector gamma-ray spectrometry at very high count rates was proposed and tested, with



Figure 2: The HEROS L3 absorption spectrum reconstructed from the $2p_{3/2}3d_{5/2}$ RIXS spectrum recorded at 4758.9 eV excitation energy compared with the $2p_{3/2}3d_{5/2}$ HERFD spectrum taken at 4110.09 eV emission energy. The total fluorescence yield (TFY) spectrum is also presented for comparison (M. Kavčič et al., Phys. Rev. B 87, 075106, 2013.)

a patent granted on the subject. The first stage of the industrial project "Extending the MPPC operation into the saturation regime" was completed.

Tritium and C-14 were the main topics in the Laboratory for Liquid Scintillation Spectrometry. The determination of tritium in different types of environmental waters for the purposes of dating and hydrological studies was upgraded with a metrological approach in a bilateral cooperation with Romanian colleagues. A comparison study of methods and scintillation cocktails for a determination of tritium in urine was performed and different approaches to handling spectra with a high level of quench were tested. A direct method for the determination of the bio components' content in fuels was improved and its range was broaden up to 100%.

The laboratory for radiological measurement systems and radioactivity measurements conducted an extensive program of radiological monitoring, including the radiological monitoring of the living environment in Slovenia, radiological monitoring of fodder in Slovenia, regular off-site radiological monitoring around Krško Nuclear Power Plant (NPP), independent radiological monitoring of the NPP, environmental monitoring around the central radioactive waste repository in Brinje, monitoring of the radioactivity in drinking water. In addition, work at the department included certified calibrations of the radiation gauges and TLD measurements of the personal and environmental doses. The laboratories active in the radiological monitoring are certified according to the ISO 17025 standard.

In the frame of the project FP7-Fission-2012 "Innovative integrative tools and platforms to be prepared for radiological emergencies and post-accident response in Europe", the task "Table-top exercise on monitoring a large-scale cross-border contamination", was organised in the period Dec. 11-12, with participants from 15 EU member states. In 2013, the department continued the collaboration with Metrology Institute of the Republic of Slovenia (MIRS) as the holders of radiological ethalon in the frame of European Metrology Research Programme (EMRP). The department is actively involved in the projects "MetroMetal: Ionising radiation metrology for the metallurgical industry", "MetroRWM: Metrology for Radioactive Waste Management" and "MetroNORM: Metrology for processing materials with high natural radioactivity". The department runs a radiological mobile unit, which performed its regular and in-field prepardeness trainings around the Nuclear Power Plant Krško. In addition, it executed a demonstration of in-field action in collaboration with Administration of the Republic of Slovenia for Civil Protection and Disaster Relief.

In the beginning of 2013 we performed one of the first measurements at the new free-electron laser Fermi (Trieste). Through an analysis of the experimental results we demonstrated for the first time the two-photon resonant excitation processes for doubly excited states of helium by the detection of metastable atom decay products. Due to its seeded mode of operation, Fermi is momentarily the only (quasi)monochromatic source of extremely intense light in the VUV energy region. After we submitted the results of our analysis of the avoided crossing experiments for singly excited states of helium in a homogeneous electric field, noting the effects in the metastable yield due to the unwanted presence of the magnetic field we have proposed and conducted another experiment at the Gasphase@Elettra beamline under the controlled presence of both the electric and magnetic field. For this purpose we built a compact "Helmholtz capacitor" that allows the setting of specific field configuration with respect to the polarization of the incoming light as well as the attenuation of unwanted field components in the target region.



Figure 3: Relative changes in CO oxidation over Pt on Co in the presence and absence of a magnetic field at 120°C. The gas flow composition is 1%CO and 2% O2 in Ar (total flow 30 mL/min). (J. Sa et al., Nanoscale 5, 8462, 2013).

We achieved a better resolution with respect to the variation of the field magnitude and the results represent the first accurate systematic study of the helium LS coupled manifold of states interacting with a homogeneous electric and magnetic field. In 2013 we collaborated strongly with French researchers from the LCPMR institute (Paris). We published a comparative study of the two core-hole decay of carbon in the molecular series C2H2, C2H4 in C2H6 to confirm the old thesis about the larger chemical sensitivity of the near-edge measurements for two core-holes situated at different atoms in the molecule (Phys. Rev. Lett. 110, 163001). In autumn 2013 we participated in first magnetic bottle experiments involving a combination of C K and Cl L hole in CCl4. We also participated at the experiment at Soleil to measure Auger spectra upon the resonant excitation of the Cl K orbital in chloromethane. In the field of molecular physics we published our first, theoretically rooted study about the dissociation of chloromethanes upon the excitation of the s* resonance from the Cl K shell observed with high-

resolution x-ray spectroscopy (J. Chem. Phys. 139, 134302). At the end of 2013 we entered the COST action CM1204: XUV/X-ray light and fast ions for fast chemistry (XLIC).

In 2013, we performed three experimental projects at the ID26 beamline of the ESRF synchrotron employing high-resolution x-ray spectroscopy. In collaboration with the University of Leuven we performed in-situ time-resolved RIXS measurements of cationic Ag clusters in zeolites during their x-ray induced formation. Using a wavelength-dispersive spectrometer and combining separate points on the homogeneous target we were able to record full L3M5 Ag RIXS maps with a 1-sec time resolution. These measurements will enable us to analyse the formation process and understand the electronic properties of the emissive Ag clusters. In the second project, which was performed in collaboration with the University of Helsinki, we have used RIXS spectroscopy at the sulphur K edge to study the local electronic structure and properties of solutions of sulphuric acid in water. These measurements will yield valuable information on the hydration of sulphuric acid on the molecular level, which plays a key role in atmospheric aerosol formation. Within the third project we performed preliminary S K edge RIXS measurements on several polysulfide samples, which are present within LiS batteries, and also three samples of LiS battery cathode material during different stages of the discharging cycle. The samples were prepared by our colleagues from the Institute of Chemistry. The measurements confirmed the high potential of RIXS spectroscopy to perform the chemical speciation of S in Li batteries and probe the S redox chemistry during the battery-charging cycle. In the field of gas-phase RIXS studies we have published in 2013 the results of the L3M5 RIXS measurements on Xe recorded at a fixed off-resonant excitation energy (Phys.

Rev. B 87, 075106). The Xe example is used to present a novel method suitable for the measurement of a high-energy resolved absorption spectrum upon target excitation with an intense monochromatic pulse of x-ray light. Using a dispersive-type emission spectrometer, the scanning is completely avoided. Such an approach enables shot-by-shot measurements and in principle allows the acquisition of a full spectrum by a single intense monochromatic x-ray pulse. We presented our work in a talk at the large biennial conference ICPEACXXVIII in Langzhou, China. Together with research colleagues from the Paul Scherrer Institute we have published the results of in-situ L3M5 RIXS experiments on non-magnetic Pt catalysts, supported on carbon-coated magnetic Go nanoparticles. The measurements revealed the change of the Pt electronic structure induced by an external magnetic field. Consequently, this changed the Pt catalytic performance and enabled the catalytic control by means of an external magnetic field (Nanoscale 5, 8462). In the field of high-resolution PIXE spectroscopy employing proton beam we have published the results of K β spectra of chlorine standards and several fine fraction aerosol samples. The measured K β spectra exhibited pronounced chemical effects, which were used to identify the chemical state of Cl in aerosol samples, demonstrating the feasibility of the high-resolution PIXE method for the chemical speciation of Cl in aerosol (Spectrochimica Acta Part B 79–80, 58).

The material properties were studied with measurements of magnetic and electric hiperfine fields using Mössbauer spectroscopy. The research was focused on cathode materials for lithium batteries, which were studied at the synchrotron facilities Petra in Hamburg and APS in Chicago. The sample structure was revealed by X-ray diffraction techniques, neutron diffraction, Mössbauer spectroscopy using 57Fe isotope and NMR spectroscopy on 6Li. Based on this results we presented a model "1Fe 2Li" on the kation distribution in LiFeBO₂.

The x-ray absorption spectroscopy research group has gained access to three beamlines (ID21, BM23 and XAFS) at ESRF (Grenoble) and Elettra (Trst) synchrotron where six experiments were performed in 2013. In collaboration with the Centre of excellence CO NOT a series of in-situ experiments were performed with XANES and EXAFS on Li-sulphur (Li2Sx) cathode materials for batteries with a high energy density. The XAS spectra were recorded during the reduction and oxidation of materials with C/15 dynamics. They register the change of valence of Mn and Fe, and the formation of Li2Sx compounds during the processes, providing the key information on the battery dynamics and opening the way to optimization of the synthesis of the material with maximum capacity. The results are presented in a paper, accepted for the publication end of 2013 and in talks on international conferences and foreign universities. We continued a long-term project, in collaboration with the Institute of Chemistry, which involves XAS measurements on the catalytic mesoporous molecular sieves doped with Ca, Cr, Mn, Fe, Ni and



Figure 4: Core-hole clock spectroscopy can be used to measure charge transfer through noncovalent interactions. For model system of 1,4-Benzenediamine molecules on a gold surface the electron transfer across the Au-donor-acceptor bond occurs in less than 500 as (G. Kladnik et al., J. Phys. Chem. C 2013, 117, 16477).



Figure 5: Thermo-adsorption of deuterium on polycrystalline tungsten sample. (a) The experimental surface deuterium areal density is shown as dots during sample cooling and exposure to the atomic deuterium beam. The modelled D areal density is shown as a line. (b) Experimental H areal density variation during D atom exposure. (c) Temperature decrease and its polynomial fit. (Markelj et al., Appl. Surf. Sci. 282, 478, 2013).



Figure 6: Sulphur K-edge XANES spectra of the Li-S battery operated in operando mode: a) in intermediate state at nominal composition Li_{0.3}S. Solid squares, experiment; magenta line, best fit with linear combination of reference XANES profiles. (Patel et al., accepted for publ. Chem. Phys. Chem.)

Cu, containing also organic building units on CuPd catalysts. The valence of dopants and their atomic neighbourhood is determined, to elucidate their catalytic properties. The materials aim at commercial applications such as molecular sieves and separators, adsorbents and ion traps, as well as solid heterogeneous catalysts sensitive to the molecular shape. One paper from this research topic was accepted for publication in 2013. In collaboration with Biotechnical Faculty of University of Ljubljana we performed four series of XAS experiments to determine the distribution of pollutant elements (Se, Hg, Cd, Zn. Ni, Cr) and essential elements (Zn. Cr, Fe) in the cells of hyperaccumulating plants (Plant, cell and environment 60, 2013). We published the analysis of Cd binding at the cellular and tissue levels (Plant and soil 370, 125) and the analysis of the pattern of iron distribution in maternal and filial tissues in wheat grains (Journal of Experimental Botany 64, 3249). A submicron monochromatic x-ray beam with a lateral resolution of 0.3 micrometre was used. The distribution of sulphur, chlorine and zinc was scanned simultaneously, to reveal correlations between the elements. The transport of the metal from the roots to stems, leaves and other tissues was elucidated, together with the molecular and cellular mechanisms which induce the tolerance to the noxious metal cations. About this research we published a book chapter (Phytotechnologies: remediation of the environmental contaminants. Boca Raton (FL): Taylor & Francis, cop. 2013, 443).

and invited us to participate. The upgrading of our vibrational spectrometer

for hydrogen molecules continued. In the field of the low-energy electronmolecule collisions we worked in collaboration with The Open University, Milton Keynes, UK, on an experimental determination of anion production from acetylene (C2H2) using 0-90 eV electrons. By evaluating the case of a Titan atmosphere we have shown the importance of the contribution of dipolar dissociation to the total anion production in planetary ionospheres

Within our collaboration at the ALOISA beamline of Elettra synchrotron (Lab. IOM/CNR), we investigated the electronic properties of organic-inorganic and hetero-organic interfaces. Within our studies of carrier transport over empty molecular orbitals in adsorbed aromatic molecules we succeeded to map the preferred pathways of ultra-fast carrier transport from organic molecules to the underlying substrate and to relate them to a specific type of molecular bonding. With the use of X-ray resonant spectroscopy we studied a model aromatic system, 1,4-benzenediamine molecules bound on

a Au surface through an Au-N donor-acceptor bond, as these are known to

provide a pathway for electronic conduction in molecular devices. We show

(paper in press in Physical Chemistry and Chemical Physics).

In collaboration with the Laboratory for material research of the University of Nova Gorica we published a paper with high impact in Chemistry of Materials about cation order-disorder transition in Fe-doped 6H-BaTiO, for dilute room-temperature ferromagnetism (Chemistry of Materials, 25, 3544).

Work within the EU's fusion development program in 2013 was focused on the three priority supported EFDA tasks in collaboration with INFLPR, Bucharest, Romania, IPP, Garching, Germany, and PIIM, Univ. Aix-Marseille, France. For all these studies the Nuclear Reaction Analysis (NRA) method was used for deuterium depth profiling in materials by using a high-energy 3He ion beam produced by a 2MV tandem accelerator at MIC. For this purpose protons from the nuclear reaction D(3He,p)4He are detected. In-situ NRA studies were performed during the thermal desorption of D from samples with D co-deposited or implanted or during D uptake on samples initially D-free but subjected to a D-atom beam (Applied Surface Science 282, 478). The studied materials were thin layers of various combinations of W, C and Al, as well as tungsten damaged by high-energy ions to simulate neutron damage (Journal of Nuclear Materials, 438, S1027). Due to the importance of this issue, IAEA has initiated in 2013 a CRP on this subject

that charge delocalization across the donor-acceptor bond occurs in less than 500 as. Furthermore, the Au-N bond also enhances delocalization to the substrate from the neighbouring carbon sites, demonstrating that fast charge transfer across a metal-organic interface does not require a covalently bonded system (J. Phys. Chem. C 117, 16477). Shape-complementarity of donor (D) and acceptor (A) molecules drives the hetero-organic self-assembly of photovoltaic elements into an extended interface with a ball-and-socket structural motif, which increases both the active volume and exciton dissociation rates to improve the efficiency of organic solar cells. Using core hole clock (CHC)



Figure 7: Interface of PDZ-01 XRF analyser, developed at the department (P. Kump and Z. Rupnik).



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X-ray spectroscopy and density functional theory (DFT), we compare the electronic coupling, and charge-transfer rates at the interface between the C60 acceptors and the flat- or contorted-hexabenzocorone (HBC) donors. This work provides fundamental mechanistic insights on the improved efficiency of organic photovoltaic devices that incorporate these concave/convex D/A materials (Advanced Energy Materials, 3, 894)

In the tandem accelerator laboratory of JSI, efforts were invested into the successful operation of a new, multicusp ion source, acquired in the frame of Large Scientific Equipment Package No. 14. After its installation, work

was dedicated to the tuning of the ion source to the requirements of the accelerator. Work was successfully accomplished. We measured the normalized brightness of the high-energy proton beam with a two-slit system and achieved the value of 14, by far the highest value ever reported on tandem accelerators. Earlier reported values did not exceed values of 4 (Pelicon et al., submitted to NIM B). With such proton beam characteristics, we are able to lower the object slit size and the acceptance angle of the quadrupole lens and correspondingly achieve a much better lateral resolution in applications with high-energy focused proton beams. The micro-PIXE method is now operating with the available lateral resolution of 800 nm. In combination with the frozen hydrated tissue-handling technology, developed in the last three years, we are able to provide top experimental conditions for the quantitative elemental mapping of biological tissue. Together with external users, several papers were published, including work on wheat (Singh et al, Jour. Exp. Bot. 2013, Pongrac et al, Jour.Roy.Soc.Int. 2013) and tartary buckwheat (Pongrac in sod., Food Res. Int. 2013). Recent work in the field of nanotoxicology resulted in a paper on the fate of cobalt after the insertion of CoFe2O4 nanoparticles in organisms (Novak et al, Env. Sci. Tech, 2013). In 2013, several researchers expressed their interest to apply micro-PIXE to study processes in brains. In collaboration with Carla Iochims and Paulo Jobim



Figure 8: In 2013, we achieved a significant progress in development of molecular imaging by MeV SIMS. Home-built Time-Of-Flight spectrometer for MeV SIMS was calibrated and imaging implemented. Graph shows mass calibration spectrum measured on arginine by excitation of 5.8 MeV chlorine ions (Jeromel et al., accepted for publication in NIM B).

from "Universidade Federal do Rio Grande do Sul", Porto Alegre, Brazil, we measured elemental distributions in rat brain tissue. Aleksandra Wandzilak from AGH University of Science and Technology, Krakow, Poland, measured the elemental distributions in human brain-tumour tissue. Important progress was achieved in the development of the MeV SIMS spectrometry, where the desorption of large unfragmented molecular ions is induced by high-energy heavy ion impact. The acquisition was developed at the field-programmable gate array (FPGA) platform, which enables multi-hit acquisition and molecular mapping. A mass resolution of 300 was achieved using a home-built Time-Of-Flight (TOF) telescope and the required steps toward the mass resolution of 1000 were indicated. We continue to provide beamtime to the researchers from the European research area in the frame of Transnational access (TNA) programme of the 7th FP EU project SPIRIT (www.spirit-ion.eu). Magali Schnell-Ramos from the University of Udine, Italy, studied iron-enrichment effects in the wheat species durum using micro-PIXE. We measured quantitative elemental maps on the cross-sections of the wheat grains with micro-PIXE. Camille Larue from Ruhr-Universität Bochum and Hiram Castillo-Mitchell from ESRF, Grenoble, applied micro-PIXE for studies of zinc and iron homeostasis in the plant Arabidopsis thaliana. With the tissue-preparation assistance by the colleagues from Biotechnical Faculty, University of Ljubljana, they measured elemental maps with micro-PIXE on frozen hydrated plant tissue. This is the first TNA project at JSI tandem accelerator done by recently developed frozen hydrated tissue technology. Within archaeometric research we studied glass and precious stones using in-air PIXE spectroscopy and complementary techniques. The emeralds from the Slovenian archaeological sites were analysed. This measurement together with mineralogical investigation showed emerald provenance in Egypt, though a small fraction of emeralds may originate from Afghanistan or some other sites in Egypt as well. In the same way we analysed the garnets, which are compositional part of the jewellery from the Migration Period. We confirmed the garnet provenance in South India and Sri Lanka, but we did not find any garnets from the European sites, which are typically applied on objects from the 7th c. AD. The explanation may be sought in the political changes in the territory of the present Slovenia, induced by Avaric and Slavic incursions in the 7th c. The glass analysis involved samples from Albania and the site Tonovcov grad in Slovenia. The glass from Albania showed several groups that could be related with different sources of raw materials. This finding supports the recent thesis that the glass from the Imperial period was produced in different places within Europe, but the production concentrated in the area of the present Palestine in Late Antiquity. Two types of late Roman glass were recognized in the inventory from Tonovcov grad, similar to the glass composition in Italy and eastern Mediterranean, but not in Western Europe.

Laboratory for x-ray fluorescence analysis applied the X-ray Florescence (EDXRF) method to analyse soil, plant samples and thin film-covered pharmaceutical pellets. EDXRF analysis was used to determine the mineral contents of P, S, Mn, Fe, and Zn for 150 sorts of Slovenian wheat. The concentration values accessed will be used for the further

XANES analysis with the synchrotron micro-beam for the purpose of studying the bioavailability of these essential nutrients. The EDXRF analysis was used to study museum artefacts, mainly weapons and armour. A method for fast identification of plastic materials was developed based on measurements of the coherent and incoherent scattering of X-rays in an EDXRF experiment. In collaboration with members of the Biotechnical Faculty we participated in experiments on the TwinMic beamline of the synchrotron Elettra in Trieste and the beamline ID 21 of synchrotron ESFR in Grenoble, where the in-house procedures and software for the quantification of XRF results was developed and used. Dr. Peter Kump constructed a prototype of the portable EDXRF analyzer.

Organization of conferences, congresses and meetings

1. Monitoring a large scale cross border contamination in the aftermath of a nuclear accident, Ljubljana, 11.–12. 12. 2013

Patent granted

1. Silvan Bucik, Borut Baričevič, Borut Repič, Matjaž Vencelj, A method of analog and digital signal processing of information contained in pulses, and a device for achieving the same, SI23959 (A), Urad RS za intelektualno lastnino, 28.6.2013.

INTERNATIONAL PROJECTS

- Services Foreign buyers Branko Vodenik, M. Sc.
- Calibrations Foreign buyers
- Matjaž Mihelič, M. Sc. 3. TLD dosimetry
- Foreign buyers Boštjan Črnič
- Provision of Testing Services for Filter Media used in IMS Radionuclide Stations CTBTO Preparatory Commission Dr. Benjamin Zorko
- 5. 7FP SPIRIT; Support of Public and Industrial Research Using Ion Beam Technology European Commission
- Asst. Prof. Primož Pelicon 6. 7FP - SPRITE; Supporting Postgraduate Research with Internships in Industry and Training Excellence
- European Commission Asst. Prof. Matjaž Kavčič
- 7FP PREPARE; Innovative Integrative Tools and Platforms to be Prepared for Radiological Emergencies and Post-accident Response in Europe European Commission Dr. Benjamin Zorko
- 7FP EÚRATOM; Application of Ion Beam Analytical Methods to the Studies of Plasma Wall Interaction Studies - 1.4.3.-FU; 3211-08-000102, FU07-CT-2007-00065 Location
 - Ministry of Education, Science and Sport
 - Asst. Prof. Primož Pelicon
- 9. 7FP EURATOM-MHEST; 1.4.1.-FU, Processes with Neutral Hydrogen Atoms and Molecules
 - Ministry of Education, Science and Sport Dr. Sabina Markelj
- 7FP EURATOM-MHEST, WP13-IPH-A03-P1-01/MESCS/PS, Atomic and Low-Energy Hydrogenic Plasma Interaction with Damaged Tungsten Ministry of Education, Science and Sport Dr. Sabina Markelj
- 7FP EURATOM-MHEST, WP13-IPH-A03-P2-01/MESCS/PS, D Re-Adsorption/Re-Saturation of W Surfaces Subject to Helium RF - Discharge as a Fuel Removal Technique Ministry of Education, Science and Sport Dr. Sabina Markelj
- 12. 7FP EURATOM-MHEST; WP13-IPH-A01-P3-01/MESCS/PS, Analyses of the Deuterium Trapping in Mixed Materials and Analyzes of Mixed Materials Films Relevent to ITER by Ion Beam Analytical Methods Jožef Stefan Institute
 - Asst. Prof. Primož Pelicon
- 13. MetroRWM; Metrology for Radioactive Waste Management Euramet e.V.
- Branko Vodenik, M. Sc.
- 14. MetroMetal Ionising Radiation Metrology for the Metallurgical Industry

Euramet e.V.

- Branko Vodenik, M. Sc. 15. MetroNORM; Metrology for Processing Materials with High Natural Radioactivity Euramet e.V. Branko Vodenik, M. Sc.
- Convention de mise a disposition; Letter N/REF: NS/MD/CONV/04FRE2681JS/2004 dtd. 8. 9. 2004
 - Ecole Normale Superieure Dr. Iztok Čadež
- Dr. Izlok Cauez
 Determination of Trace Elements in Lu Foil by k0-INAA and XRF
- Institute for Reference Materials and Measurements Dr. Peter Kump
- COST CM1204: XUV/X-ray Light and Fast Ions for Ultrafast Chemistry (XLIC) COST Office
 - Asst. Prof. Matjaž Žitnik
- IAEA Fellowship for Ms Aleksandra Wandzilak, POL/13005 IAEA - International Atomic Energy Agency Asst. Prof. Primož Pelicon
- Hydrogen Retention in Self-damaged and He Irradiated Tungsten Alloys in Fusion Devices; Plasma-Wall Interaction for Irradiated Tungsten and Tungsten Alloys in Fusion Devices
 LAFA - International Atomic Energy Agency
 - IAEA International Atomic Energy Agency Dr. Sabina Markelj
- Preparation and Analysis of Reference Materials Iarma Limited
- Dr. Jasmina Kožar Logar 22. Different Analyses
- 22. Different Analyses Foreign buyers
- Dr. Jasmina Kožar Logar
- 23. Dynamics at Nanoscale
- Slovenian Research Agency Asst. Prof. Matjaž Žitnik
- LSC Methods for Determination of H-3 and C-14 in Environmental Samples Slovenian Research Agency Dr. Jasmina Kožar Logar
- Study of Deeply Virtual Compton Scattering Slovenian Research Agency Perof Simon Simon
- Prof. Simon Širca 26. Virtual Compton Scattering on the Nucleon Slovenian Research Agency
- Slovenian Research Agency Prof. Simon Širca 27. Measurements and Control of Deutorium in D
- Measurements and Control of Deuterium in Fusion Material Slovenian Research Agency Asst. Prof. Primož Pelicon
- Co-financing of the Promotion of Science European Commission
 - Asst. Prof. Primož Pelicon

RESEARCH PROGRAMS

- 1. Archaeological and Archaeometric Research of Portable Archaeological Heritage Prof. Žiga Šmit
- 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 Asst. Prof. Matjaž Žitnik

R&D GRANTS AND CONTRACTS

- Investigation of Plant Ion Homeostasis Using Elemental Imaging by Laser Ablation -Inductively Coupled Plasma Mass Spectrometry (Basic Research Project) Asst. Prof. Primož Pelicon
- 2. Research of the Ionome of Selected Mycorrhizal Plants
- Asst. Prof. Primož Pelicon
- Sustainable Land Use in Relation to Soil and Crop Quality Asst. Prof. Primož Pelicon
- 4. Archaeologies of Hunter-Gatherers, Farmers and Metallurgists: Cultures, Populations, Palaeoeconomies and Climate
- Dr. Marijan Nečemer 5. Nanostructured Cathodes for Lithium Sulphur Batteries Dr. Darko Hanžel
- 6. Groundwater Age Determination in Deep Aquifers of Slovenia
- Dr. Jasmina Kožar Logar 7. Complex Hyperspectral System for Automatic Analysis and Control of Pharmaceutical Pellet Coating Processes
- Dr. Peter Kump
 8. The Use of Specific Methods for Determination and Prevention of Adulteration of Milk and Dairy Products
 Dr. Marijan Nečemer

VISITORS FROM ABROAD

- 1. Dr. Margarita Herranz Soler and Dr. Raquel Iodeta, ETSI, Bilbao, Spain, 13.-17. 1. 2013
- 2. Antti Kettunen, Oulu University, Oulu, Finland, 6. 5.-17. 6. 2013
- Assoc. Prof. Osman Şahin, Asst. Prof. Bünyamin, Asst. Prof. Sinan Yaşar, Mustafa Kemal University, Hatay, Turkey, 3.–8. 6. 2013
- 4. Martine Schulte-Borchers, ETH, Zürich, Switzerland, 4.-6. 6. 2013
- 5. Dr. Camille Larue, Ruhr-University Bochum, Bochum, Germany, 8.-12. 7. 2013
- 6. Dr. Hiram Castillo-Michel, ESRF, Grenoble, France, 8.-12. 7. 2013
- Dr. Carmen Varlam, Dr. Ionut Faurescu, INC-DTCI-ICSI, Ramnicu Valcea, Romania, 25. 8.–7. 9. 2013
- 8. Dr. Dimosthenis Sokaras, SSRL, Menlo Park, USA, 8.–12. 9. 2013
- Dr. Helene Fonvieille, Loup Correa, CNRS, LPC Clermont-Ferrand, Clermont-Ferrand, France, 15.–20. 9. 2013

- Center of Competence BioMedical Engineering: CC BME Dr. Matjaž Vencelj
- EMRP MetroRWM; Metrology for Radioactive Waste Management Branko Vodenik, M. Sc.
- 11. EMRP MetroMetal; Ionising Radiation Metrology for the Metallurgical Industry Branko Vodenik, M. Sc.

NEW CONTRACTS

- Monitoring of Radioactivity in the Living Environment in Slovenia 2013-2014 Ministry of Agriculture and the Environment Dr. Benjamin Zorko
- Extension of MPPC Performance into the Saturation Regime Beyond Devices, d. o. o.
- Dr. Matjaž Vencelj
- 3. Support to Research Work of Industrial Young Researcher Romana Krištof in 2013 Ames, d. o. o.
- Dr. Jasmina Kožar Logar 4. Off-site Radiological Monitoring of NPP Krško 2011-2013
- Krško Nuclear Power Plant Doc. dr. Matej Lipoglavšek
- Annex No. 7 to the contract on performing activities and fulfillment of obligations of holder of national standard in the field of ionising radiation Ministry of Economic Development and Technology Mag. Denis Glavič Cindro
- 6. Ecology laboratory with mobile unit 2013 Ministry of Defence Asst. Prof. Matej Lipoglavšek
- Aleksandra Wandzilak, Faculty of Physics and Applied Computer Science AGH, Kraków, Poland, 23. 9.–22. 12. 2013
- 11. Dr. Dolors Company, University of Girona, Girona, Spain, 29. 9.-6. 10. 2013
- 12. Dr. Carla Iochims , UFGRS, Porto Alegre, Brazil, 4.-14. 10. 2013
- 13. Dr. Paulo Jobim, UFGRS, Porto Alegre, Brazil, 4.-25. 10. 2013
- 14. Abdulghani Shakhashiro, IARMA Limited, Thurso, UK, 24.-30. 10. 2013
- 15. Marlina Harnisch, Katrin Tanzer, IPP, Innsbruck, Austria, 4.-15. 11. 2013
- 16. Prof. Claudio Spitaleri, INFN and LNS, Catania, Italy, 5.-7. 11. 2013
- Giuliano Mini, Giovanni Burgada, CAEN SpA, Viareggio Lucca, Italy, 12.–13. 11. 2013
- 18. Lukaš Skala, ENVINET as, Trebic, Czech Republic, 12.–13. 11. 2013
- 19. Giscard Honore Sonkwa Monthe, University of Yaoundé, Yaoundé, Cameroon, 1.-23. 12. 2013
- 20. Dr. Régis Bisson, Aix Marseille University, Marseille, France, 17.-20. 12. 2013

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Researchers

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- 9. Prof. Andrej Likar*, retired 01.10.13
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- 24. Luka Jeromel, B. Sc.
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- 38. Zvonimir Grabnar
- 39. Mirko Ribič, B. Sc.

Note: * part-time JSI member

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ORIGINAL ARTICLE

- 1. A1 Collaboration, Patrick Achenbach *et al.*, "Overview of the electromagnetic production of strange mesons at MAMI", V: XI International Conference on Hypernuclear and Strange Particle Physics, HYP2012, Barcelona, Spain, 1-5 October 2012, *Nucl. Phys. A*, vol. 914, pp. 41-50, 2013.
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- 4. Hermann Bothe, Katarina Vogel-Mikuš, Paula Pongrac, Matevž Likar, Neva Stepic, Primož Pelicon, Primož Vavpetič, Luka Jeromel, Marjana Regvar, "Metallophyte status of violets of the section Mellanium", *Chemosphere (Oxford)*, vol. 93, issue 9, pp. 1844-1855, 2013.
- 5. Mirela Dragomir, Iztok Arčon, Sandra Gardonio, Matjaž Valant, "Phase relations and optoelectronic characteristics in the NdVO4-BiVO4 system", *Acta mater.*, vol. 61, no. 4, pp. 1126-1135, Feb. 2013.
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- 11. Ebrahim Gholami Hatam, Mohammad Lamehi-Rachti, Primož Vavpetič, Nataša Grlj, Primož Pelicon, "Surface topography of 1 eur. coin measured by stereo-PIXE", In: Proceedings of the 13th International Conference on Nuclear Microprobe Technology, 22-27 July 2012, Lisbin, Portugal, *Nucl. Instrum. Methods Phys. Res., Sect. B*, vol. 306, pp. 90-93, 2013.
- 12. Denis Glavič-Cindro, Ljudmila Benedik, Jasmina Kožar Logar, Branko Vodenik, Benjamin Zorko, "Detection of Fukushima plume within regular Slovenian environmental radioactivity surveillance", In: Proceedings of the 6th International Conference on Radionuclide Metrology Low Level Radioactivity Measurement Techniques, 17-21 September 2013, Jeju Island, Korea, *Appl. Radiat. Isot.*, vol. 81, pp. 374-378, 2013.
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- Matjaž Kavčič, Matjaž Žitnik, Klemen Bučar, Andrej Mihelič, Bor Marolt, J. Szlachetko, P. Glatzel, K. Kvashnina, "Hard x-ray absorption spectroscopy for pulsed sources", *Phys. rev., B, Condens. matter mater. phys.*, vol. 87, no. 7, pp. 075106-1-075106-6, 2013.
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- 20. Matjaž Korun, Branko Vodenik, Benjamin Zorko, "Evaluation of gammaray spectrometric results near the decision threshold", *Appl. radiat. isotopes*, vol. 73, pp. 1-8, 2013.
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INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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PATENT APPLICATION

1. Matjaž Vencelj, Matej Lipoglavšek, Rok Uršič, *A device to determine the photon interaction depth in a scintillating material*, P-201300428, Urad RS za intelektualno lastnino, 16.12.2013.

PATENT

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MENTORING

- 1. Jelena Gajević, *Electron screening in nuclear reactions:* doctoral dissertation, Ljubljana, 2013 (mentor Andrej Likar).
- 2. Boštjan Drolc, *Initiating independent monitoring of quality of gamma-cameras in Slovenia:* master's thesis, Ljubljana, 2013 (mentor Andrej Likar; co-mentor Gregor Omahen).
- 3. Alberto Sànchez Ortiz, *Algorithms for digital pulse processing:* master's thesis, Ljubljana, 2013 (mentor Matej Lipoglavšek; co-mentor Matjaž Vencelj).
- 4. Urška Gradišar, Thermoluminescence analysis of irradiated food: master's thesis, Ljubljana, 2013 (mentor Žiga Šmit; co-mentors Benjamin Zorko, Katarina Vogel-Mikuš and Marijan Nečemer).
- Tina Vodopiveć, Liquid Scintillation Spectrometry and Tritium in Urine: master's thesis, Ljubljana, 2013 (mentor Matej Lipoglavšek; co-mentor Jasmina Kožar Logar).

DEPARTMENT OF THIN FILMS AND SURFACES

F-3

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

In the past few years the trendline of hard coating research has been concentrated into nanostructured coatings, i.e. nanolayer and nanocomposite coatings. The (Ti,Al,Si)N-based coatings are distinguished by the possibility to form 10-nm-sized TiN or TiAlN grains in a matrix of amorphous Si₂N₆₀ provided the proper deposition conditions are met. A year ago we implemented this coating in industrial production; today it is in regular use by about 20 companies in Slovenia. Nevertheless, we are still engaged in its characterization and interpretation. Using transmission electron microscopy we analysed the coatings at the nanolevel (nanograin size and orientation), we explained the Head (since 1.3.2013): growth mechanisms and specific features of nanograin formation in nanolayer and nanocomposite coatings. This Asst. Prof. Miha Čekada contribution was made by Aleksandar Miletić (University of Novi Sad, Serbia), which is the topic of his Ph.D thesis; he made most of the experimental work in our department.



We analysed the (Ti,Al,Si)N coating in semi-industrial experiments, where wear mechanisms in hard milling were studied in controlled conditions. The tools were either coated by a nanocomposite, or by one of the standard coatings for reference. A part of these tests was performed in the scope of the Nano-tool project (ERA-SME, partners Vienna Technical University and company EMO Orodjarna, d. o. o.). A series of experiments with a systematic evaluation and special emphasis on wear was performed by Dr. Halil Çalişkan from the University of Bartin, Turkey. He worked on this topic in the scope of his one-year stay in our department as part of his Ph.D thesis.

The appearance of micrometre-size growth defects is one of the major problems in the application of hard coatings. In this year we paid specific attention to those defects that originate in errors in the base material. We found that a lot of defects form on non-metal inclusions, which are found in all steels; this mainly applies to oxides (e.g. SiO₂) and sulphides (MnS). Their sputtering rate during etching is very different; therefore, in the phase of ion etching topographic changes on the surface appear. In the scope of the ESTEEM-2 project we were awarded session time in a high-resolution transmission electron microscope at the University of Graz, Austria. The samples were prepared by focused ion beam. Using this instrumentation we were able to analyse the contact between a non-metal inclusion and the coating grown above the inclusion. We evaluated the size of the micropores, which are the origin of poor adhesion on defects. With a systematic evaluation of the surface topography after cleaning, after etching and after coating deposition, we performed a statistical estimation of the defect appearance in different phases of depositing a hard coating. This work is performed in collaboration with the Faculty of Mechanical Engineering of the University of Maribor; it is the topic of the Ph.D thesis of Peter Gselman, our young researcher. Because our research group is one of the world's leading in the topic of growth-defect diagnostics, our co-worker Dr. Peter Panjan had an invited lecture at the International Conference of Metallurgical Coatings and Thin Films in San Diego, USA.

Research is performed on several applied projects, which are cofinanced by various companies. We started the development of multicomponent coatings for the protection of tools for hot forging, produced by the company Unior, d. d. The basic idea is in the addition of vanadium, which acts as a lubricant in high-temperature conditions. We performed several experiments using the so-called triangular targets made of two elements, which enables the deposition of a vertical composition gradient. So far we analysed the systems Cr.Al, N and Cr.V. N. Going the classic way (using monolithic targets), 20 individual depositions would be needed, while by applying the triangular targets only one deposition was necessary. The use of this method is the Ph.D topic of our young researcher Aljaž Drnovšek. He thoroughly analysed the thus prepared Figure 1: SiO, inclusion in stainless steel at various samples from the tribological point of view and systematically analysed the influence of differ- steps of coating preparation



We investigated the influence of various nonmetallic inclusions in steel substrates on the mechanism of growth defect evolution.



Figure 2: Cross-section through a TiAlN/CrN multilayer structure at the position of MnS inclusion, obtained using transmission electron microscopy



Figure 3: A partly delaminated defect on a TiAlN coating

We showed that during magnetron sputtering the ionisation zones play a major role in the transport of ions and electrons. ent parameters on friction and wear. The ambient atmosphere choice (air, oxygen, nitrogen) was shown to have a major influence on the tribological properties of selected coatings.

In the previous years our tribological efforts were mainly limited to hard, self-lubricating coatings of diamond-like carbon. However, in collaboration with the company Nanotul, d. o. o., we initiated a project for testing the lubricating properties of standard coatings in combination with lubricants based on MoS_2 nanotubes. Other project-based collaborations are on-going with the companies Impol, d. d. (low-temperature coatings for aluminium alloys), Phos, d. o. o. (coatings on tools for pharmaceutical industry) and Kovinos, d. o. o. (coatings on cutting tools for hard machining).

There are several cases of collaboration, where the choice of a proper coating is only one aspect in a broad goal of the optimization of a certain technological process. One case deals with applying the TiAlN coating on highspeed steel after a cryogenic treatment (in collaboration with the University of Zagreb, Croatia), and another one with the protection of aluminium hotextrusion tools by CrN coating (in collaboration with the Faculty of Natural Sciences and Technologies, University of Ljubljana).

The collaboration with the companies often continues after the expiry of a project. The work is usually done as an investigation, where we solve specific advanced technological problems. For the company Kolektor, d. d., we are developing a coating with a purpose to improve the tribological properties of saw blades that are used to cut commutator bodies. There is an intensive collaboration with the company Cetis, d. d., where our young researcher from the industry Vladan Mladenovič is employed. The topic of his research is surface structuring with various surface-treatment techniques (scratching, laser ablation, micromilling, electroerosion), and the the analysis of these processes at microlevel. So far he has systematically analysed the topics of scratching and partly laser treatment, using the Taguchi method of experiment design.

In evaluating the degradation of functional materials, there are two well-established groups of tests. The first is the tribological testing where we evaluate the mechanical wear of two materials in sliding contact. The other is the corrosion testing where we are following the chemical destruction of the material in (mechanically speaking) static conditions. A synthesis of both concepts is the tribo-corrosion test, where we simultaneously measure the parameters of sliding wear (e.g., friction coefficient) and electrochemical parameters (corrosion potential, corrosion current). In this way we can in-situ evaluate the coating's degradation. The applicability of this principle was shown on two coatings (TiAgN and TiSiN).

In the scope of basic and industrial research we have been investigating for several years the influence of rotation on thin-film growth. Using a simulation that we developed for the industrial sputtering apparatus CC800/9 we studied the influence of rotation and target configuration on the structure of multilayer coatings and on the homogeneity of thin films. The simulation results showed that very periodic rotation modes, which depend on the turntable gear ratio, cause large variations both in thickness and in chemical composition of the coatings. Fewer periodic modes of rotation improve the film homogeneity, even though in certain rotating parameters large fluctuations may appear. Such simulations are a useful tool for the design of new PVD coatings. Our simulation attracted considerable attention from research and industry and led to the signing of a contract with one of the largest producers of PVD systems from Germany. This was also a topic of an invited lecture that our co-worker Dr. Matjaž Panjan had at the Society of Vacuum Coaters annual meeting in Providence, USA.

In collaboration with co-workers from Lawrence Berkeley National Laboratory (USA), Dr. Matjaž Panjan published a paper in Applied Physics Letters, where they proposed a model for the transport of ions in high-power impulse magnetron sputtering. The model is based on the discovery of plasma structures called ionisation zones, which rotate in the magnetron plasma in the direction $E \times B$. In this model they proposed that inside the ionization zones the electron and ion densities are spatially separated; therefore, the electric field forms in an azimutal direction. Thus, the electric field rotates in line with the zones. The ions primarily form within the ionization zones; therefore, they acquire the kinetic energy of the rotating electric field that accelerates them in the azimutal direction up to an energy of 100 eV or more. This model is supported by experiments, conducted using mass and energy spectrometry in the scope of his post-doctoral stay in Berkley.

In this year Dr. Matjaž Panjan was a visiting researcher at the Montreal Polytechnic, Canada. He continued the work on nanocomposite hard coatings prepared by high-power impulse magnetron sputtering, already started in the scope of the post-doctoral stay in Montreal. The nanocomposite TiSiN coatings were tested for the protection of turbine blades against water erosion. These tests were conducted in collaboration with Rolls-Royce Canada. The coatings reduced the wear of blades by a factor of four. Within the COST action (topic: high power impulse magnetron sputtering) our young researcher Aljaž Drnovšek visited the same lab.

Within the Euratom project our task is the synthesis of hydrogenated carbon deposits, which should be as similar as possible to real impurity deposits in a fusion reactor. We keep informal collaboration with the Institute Vinča (Belgrade, Serbia) where we prepare various multilayer coatings (Ni/ Ti, Al/Ti) to be laser-treated by our partners. Specially interesting results were obtained by the CrVN coating where we were able to synthesise a macroscopic wavy structure on the irradiation spots.

Some outstanding publications in the past year

- 1 Kek-Merl, D.; Panjan, P., Kovač, J.: Corrosion and surface study of sputtered AlW coatings with a range of tungsten contents, Corrosion science, 69 (2013), 359-368
- 2 Panjan, P., Gselman, P., Kek-Merl, D., Čekada, M., Dražić, G., Bončina, Figure 5: Image of ionization zones in high-power impulse magnetron T., Zupanič, F.: Growth defect density in PVD hard coatings prepared by different deposition techniques, Surface & coatings technology, 237 (2013), 349-356



Figure 4: Surface of a CrVN coating after oxidation (750 °C, 2 min)



sputtering, obtained with a high-speed camera

Panjan, M.: Influence of substrate rotation and target arrangement on the periodicity and uniformity of layered 3 coatings, Surface & coatings technology, 235 (2013), 32-44

INTERNATIONAL PROJECTS

- Simulation of Coating Deposition in Industrial PVD Systems 1. CemeCon AG Dr. Matiaž Panian
- 7FP EURATOM; Plasma Deposition of H:C-metal Coatings 1.4.5.-FU 3211-08-000102, 2. FU07-CT-2007-00065 Ministry of Education, Science and Sport
 - Dr. Peter Panjan

RESEARCH PROGRAM

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

R&D GRANTS AND CONTRACTS

- Organic-Inorganic Thin Film Structures for Electronics Components Dr. Peter Panjan
- Research and Development of Rapid Production and Repair in Modern 3D Cutting Tools 2.

with Advanced Laser Technologies Dr. Peter Panjan

- Protected Permanent Magnets for Advanced High-Temperature Applications 3 Asst. Prof. Miha Čekada
- 4. Multifunctional Nanostructured Films for Artificial Implants - Corrosion and Tribocorrosion Processes Dr. Darinka Kek Merl
- Colour, Absorption and Protective Nanolayer Coatings for Aluminium Alloy 5 Dr. Peter Panjan
- 6. Functionalization of Biomedical Samples by Thermodynamic Non-equilibrium Gaseous Plasma Dr. Peter Panjan
- Toward Ecologically Benign Alternative for Cleaning of Delicate Biomedical Instruments Dr. Peter Panjan
- Self-lubricating and Wear Resistant PVD Hard Coatings Based on (V, Cr, Al, Ti)N for Hot-working Processes Dr. Peter Panjan
- Reduction of Friction and Tool Wear Using Advanced Lubricants and Protective PVD Coatings

Dr. Srečko Paskvale

NEW CONTRACTS

Study of functional properties of PVD-hard coatings in the system (Cr,Al)N 1 Kovinos d. o. o. Dr. Peter Panian

VISITORS FROM ABROAD

Dr. Christoph Schiffers, CemeCon AG, Würselen, Germany, 6. 11. 2013 1. Dr. Robert Franz, Dr. Marisa Figueiredo, Montanuniversität Leoben, Leoben, Austria, 2. 21.-22. 11. 2013

STAFF

Researchers

- Asst. Prof. Miha Čekada, Head
- Dr. Darinka Kek Merl

Dr. Peter Panjan Postdoctoral associates

- 4. Dr. Matjaž Panjan
- 5. Dr. Srečko Paskvale

BIBLIOGRAPHY

ORIGINAL ARTICLE

- 1. André Anders, Matiaž Panjan, Robert Franz, Joakim Andersson, Pavel A. Ni, "Drifting potential humps in ionization zones: the propeller blades of high power impulse magnetron sputtering", Appl. phys. lett., vol. 103, no. 14, pp. 144103-1-144103-4, 2013.
- 2. Matej Babič, Jože Balič, Matjaž Milfelner, Igor Belič, Peter Kokol, Milan Zorman, Peter Panjan, "Robot laser hardening and the problem of overlapping laser beam", Adv produc engineer manag, vol. 8, no. 1, pp. 25-32, 2013.
- 3. Matej Babič, Peter Panjan, Peter Kokol, Milan Zorman, Igor Belič, Timotej Verbovšek, "Using fractal dimensions for determination of porosity of robot laser-hardened specimens", International journal of computer science issues, vol. 1, issue 2, pp. 184-190, 2013.
- 4. Halil Çalişkan, Azmi Erdoğan, Peter Panjan, Mustafa Sabri Gök, Abdullah Cahit Karaoğlanli, "Micro-abrasion wear testing of multilayer nanocomposite TiAlSiN/TiSiN/TiAlN hard coatings deposited on AISI H11 steel", Mater. tehnol., vol. 47, no. 5, pp. 563-568, 2013.
- 5. Halil Çalişkan, Cahit Kurbanoğlu, Peter Panjan, Miha Čekada, Davorin Kramar, "Wear behavior and cutting performance of nanostructured hard coatings on cemented carbide cutting tools in hard milling", Tribol. int., vol. 62, pp. 215-222, 2013.
- 6. Halil Çalişkan, Cahit Kurbanoğlu, Peter Panjan, Davorin Kramar, "Investigation of the performance of carbide cutting tools with hard coatings in hard milling based on the response surface methodology", *Int. j. adv. manuf. technol.*, vol. 66, no. 5-8, pp. 883-893, 2013. 7. Peter Gselman, Peter Panjan, "Mikrostrukturne nepravilnosti trdih
- PVD-prevlek", Vakuumist, vol. 33, no. 4, pp. 11-22, 2013.
- 8. Darja Kek-Merl, Peter Panjan, Miha Čekada, Peter Gselman, Srečko Paskvale, "Tribocorrosion degradation of protective coatings on stainless steel", *Mater. tehnol.*, vol. 47, no. 4, pp. 435-439, 2013. 9. Darja Kek-Merl, Peter Panjan, Janez Kovač, "Corrosion and surface
- study of sputtered AIW coatings with a range of tungsten contents", Corros. sci., vol. 69, pp. 359-368, 2013.
- 10. Darja Kek-Merl, Peter Panjan, Ingrid Milošev, "Effect of tungsten content on properties of PVD sputtered Al-Wx alloys", Surf. eng., vol. 29, no. 4, pp. 281-286, 2013.
- 11. Matjaž Panjan, "Influence of substrate rotation and target arrangement on the periodicity and uniformity of layered coatings", Surf. coat. technol., vol. 235, pp. 32-44, 2013.
- 12. Peter Panjan, Peter Gselman, Darja Kek-Merl, Miha Čekada, Matjaž Panjan, Goran Dražić, Tonica Bončina, Franc Zupanič, "Growth defect density in PVD hard coatings prepared by different deposition

- Self-lubricating and wear resistant PVD hard coatings based on (V.Cr.Al, Ti)N for hotworking processes UNIOR Blacksmith Industry, d.d. Dr. Peter Panjan
- Aleksandar Miletić, University of Novi Sad, Novi Sad, Serbia, 22. 7.-2. 8. 2013 3. Dr. Corneliu Porosnicu, National Institute for Laser, Plasma and Radiation Physics, Bucharest, Romania, 9.-10. 10. 2013

Postgraduates

Aljaž Drnovšek, B. Sc.

Peter Gselman, B. Sc. Technical and administrative staff

- Jožko Fišer 8.
- Damjan Matelič
- 10. Andrei Mohar
- 11. Tomaž Sirnik

techniques", In: Proceedings of the 40th International Conference on Metallurgical Coatings and Thin Films, 29 April 3 - May 2013, San Diego, California, Surf. Coat. Technol., vol. 237, pp. 349-356, 2013.

- 13. Suzana Petrović, Davor Peruško, Branislav Salatić, Iva Bogdanović-Radović, Peter Panjan, Biljana Gaković, Dejan Pantelić, Milan Trtica, Branislav Jelenković, "Laser induced damage/ablation morphology on the 8(Al/Ti)/Si system in different ambient conditions", Opt. Laser Technol., vol. 54, pp. 22-29, 2013.
- 14. Suzana Petrović, Branislav Salatić, Davor Peruško, Iva Bogdanović-Radović, Miha Čekada, Biljana Gaković, Dejan Pantelić, Milan Trtica, Branislav Jelenković, "Laser-induced structural and composition modification of multilayered Ni/Ti thin film in air and liquids", Laser phys., vol. 23, no. 2, pp. 026004-1-026004-10, 2013.

PUBLISHED CONFERENCE CONTRIBUTION

- 1. Matej Babič, Peter Kokol, Matjaž Milfelner, Peter Panjan, Igor Belič, "Use algorithm for construction 3D visibility graphs to describe plastic and elastic deformation of robot laser hardened specimens", In: Proceedings, Miroslav Babić, ed., Slobodan Mitrović, ed., Kragujevac, Serbian Tribology Society, Faculty of Engineering, cop. 2013, pp. 348-350
- 2. Matej Babič, Peter Kokol, Matjaž Milfelner, Peter Panjan, Igor Belič, "Use fractal geometry to describe friction of robot laser hardened specimen", In: Proceedings, Miroslav Babić, ed., Slobodan Mitrović, ed., Kragujevac, Serbian Tribology Society, Faculty of Engineering, cop. 2013, pp. 351-354.
- 3. Matej Babič, Peter Kokol, Matjaž Milfelner, Peter Panjan, Igor Belič, "Use new process in robot laser hardening to decrease wear of specimens", In: Proceedings, Miroslav Babić, ed., Slobodan Mitrović, ed., Kragujevac, Serbian Tribology Society, Faculty of Engineering, cop. 2013, pp. 355-358
- 4. Matej Babič, Peter Kokol, Milan Zorman, Marko Marhl, Peter Panjan, Igor Belič, Matija Lokar, Andrej Mrvar, Matjaž Milfelner, "Analyze topographical properties of robot laser hardened specimens with topological properties of visibility graphs", In: Zbornik, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 96-97.
- 5. Aleksander Drenik, Alenka Vesel, Miran Mozetič, Peter Panjan, "Recombination of atomic oxygen and hydrogen on amorphous carbon", In: Proceedings of the 15th International Conference on Fusion

Reactor Materials, October 16-21, 2011, Charleston, SC, (Journal of nuclear materials, vol. 442, no, 1/3, suppl. 2013), Amsteram, North-Holland, 2013, vol. 442, no. 1/3, suppl. 1, pp. S751-S754, 2013.

- 6. Peter Fajfar, Peter Panjan, Goran Kugler, Milan Terčelj, "Some reasons for decreased service time of dies for Al hot extrusion", In: Surface effects and contact mechanics XI: computational methods and experiments, (WIT transactions on engineering sciences, Vol. 78), J. Th. M. De Hosson, ed., Carlos Alberto Brebbia, ed., Southampton, WIT Press, cop. 2013, pp. 193-204.
- 7. Vladan Mladenovič, Miha Čekada, Peter Panjan, "Characteristics of grooving by diamond needle-tip with various tip shapes and grooving

parameters", In: *Conference & Expo 2013: technical proceedings of the 2013 NSTI Nanotechnology Conference & Expo - Nanotech 2013, May 12-16, 2013, Washington, DC*, [S. l.], TechConnect, zv. 2. 8. Sanja Šolić, Peter Panjan, "Influence of deep cryogenic treatment of the

8. Sanja Šolić, Peter Panjan, "Influence of deep cryogenic treatment of the HSS substrate on the PVD TiAlN coating properties", In: *Proceedings*, 2nd Mediterranean Conference & New Challenges on Heat Treatment and Surface Engineering, 11-14 June 2013, Dubrovnik - Cavtat, Croatia, Božidar Smoljan, ed., Božidar Matijević, ed., Zagreb, Croatian Society for Heat Treatment and Surface Engineering - CSHTSE, 2013, pp. 143-150.

DEPARTMENT OF SURFACE ENGINEERING AND OPTOELECTRONICS **F-4**

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

Non-equilibrium gaseous plasma is a suitable medium for tailoring the surface properties of hydrocarbons. These materials, especially when fibrous, may interact strongly with reactive gaseous particles, causing localized heating and thus a loss of treatment uniformity. A method for diminishing such effects is the application of a uniform gaseous plasma with a very low power density. Such a plasma is created at low pressure, which allows for the Head: minimization of three-body collisions. The collision frequency depends slightly on the type of gas and the kinetic Prof. Miran Mozetič temperature, but with a major dependence is on the gas pressure. The frequency often increases as the square of the gas pressure and in a rough approximation the value of 1 s⁻¹ is achieved at a pressure of several 10 Pa. Plasma of low power density cannot be sustained in small chambers due to the rapid diffusion of reactive particles towards the walls where they tend to be lost by neutralization, recombination and relaxation.



The characteristics of gaseous plasma were studied in an industrial scale reactor of volume 3 m³. At a pressure of 13 Pa the plasma was sustained at a discharge power as low as 50 W. The discharge power density was therefore less

than 20 W m⁻³. Just for comparison, the minimal power density for sustaining plasma created by our surfatron discharge at the same vacuum level is over 10⁷ W m⁻³. Plasma in the large reactor was created by asymmetric capacitive coupled radio-frequency discharge. The powered electrode was immersed into the centre of the reactor, while the chamber walls made from stainless steel were grounded. Since the surface of the powered electrode was well

over two orders of magnitude smaller than the surface of the grounded chamber, practically all the applied voltage appeared next to the powered electrode. The gas therefore remained at room temperature although the ionization and dissociation fractions of the gaseous molecules were reasonably high, of the order of 10^{-6} and 10^{-3} , respectively, corresponding to densities of 10¹⁶ and 10¹⁹ m³. Such a plasma is suitable for the treatment of fibrous polymer materials,

such as textiles and allows for rapid functionalization with polar functional groups as well as the removal of surface impurities. A mild plasma created in oxygen or air, however, does not allow for a dramatic increase of surface morphology, so other reactive gaseous media should be used to obtain an extremely nanostructured surface of cellulose fibres.

The textile industry in developed countries is confronting the world's marketing conditions and competitive challenges that are driving it towards the development of advanced, highly functional textiles and textiles with higher added value. The conventional textile finishing techniques are wet chemical modifications where water and rather hazardous chemicals are used in large quantities and waste waters need to be processed before discharging the effluent, whereas the most problematic factors are ecological impacts to the environment and effects on human health. The increasing environmental concerns and demands for an environmentally friendly processing of textiles leads to the development of new technologies based on the modification of functional properties with nanoparticles. Such textiles exhibit improved radiation protection, bacteriostatic effects or improved flame-retardation. A major scientific concern about the application of nanoparticles is poor adsorption onto polymer fibres, which is due to a poor Figure 1: The ionization and dissociation fractions of oxygen molecules surface morphology. Although plasma created in air, oxygen, water vapour in plasma created in 3 m3 large reactor versus distance from the wall.

Excellent functional properties for fibrous cellulose materials were achieved by the proper selection of plasma parameters.





Figure 2: SEM image of cellulose fibres treated in moist CF_{4} plasma.



Figure 3: Optical spectra of plasma created in unloaded reactor in pure CF_4 (red curve) and reactor loaded with cellulose fabrics.



Figure 4: Average wetting rise curves for non-treated and plasma treated non-woven viscose for three different liquids.

or carbon dioxide allows for a stripped, cleaned and more distinct macrofibril structure, it does not ensure the optimal adsorption of nanoparticles.

A method for the treatment of cellulose fibres that allows for almost optimal nano-structuring has been invented. The textiles were treated with a plasma created in tetraflourmethane (CF_4) with an admixture of water vapour (H₂O) in order to obtain an extremely rich surface morphology. The right treatment parameters allowed for etching resulting in a nanostructured surface with grain dimensions of roughly between 150 and 500 nm. The surface texture was uniform on a large area allowing for excellent absorption properties. The CF4 plasma is otherwise applied to obtain the opposite effect (hydrophobicity) but the right admixture of water vapour allowed for the creation of reactive particles that lead to extremely selective etching of cellulose fibres. Since the dissociation energy of a water molecule is several times lower than of CF_4 the O and OH radicals abound in plasma created in such a gas mixture and readily interact with fluorinated cellulose materials, causing etching of fluorine-rich segments. The etching was monitored using optical emission spectroscopy. The optical spectrum of plasma created in rather pure CF₄ is rich in CF₅ bands as well as continua especially in the near-ultraviolet range of wavelengths. In the case the plasma reactor is loaded with wet cellulose fabrics the optical spectrum is completely different. Instead of the CF_x spectral features the spectrum revels an extremely strong emission that originates from the transitions of CO radicals. These radicals are formed upon the etching of cellulose material with gaseous plasma created in CF₄ gas with admixture of water vapour.

Wounds are considered as the major cause of morbidity and impaired quality of life, especially by patients suffering from diabetes. It has been estimated that over 1% of the world's population suffer from serious complications causing chronic ulcer wounds. The average cost of a treatment cycle is estimated to about €6600 for leg ulcers and €10,000 for foot ulcers. Wound dressings are regarded as the medical means of cleaning and protecting wounds in order to facilitate and accelerate the healing process. Although the healing process of wounds is a natural process, the speed of healing and fluid loss is still one of the major challenges. Significant improvements in developing wound-dressing products have been recorded since earliest times, but the properties of those materials currently used are still far from challenging the characteristics that chronic wounds exhibit. In order to improve the sorption kinetics of non-woven viscose materials, nowadays widely used as absorption material, we optimized the plasma parameters for the deep functionalization of such fibrous materials. Since charged particles are lost by neutralization on the fibres' surface we rather treated these materials with an extremely non-equilibrium plasma created in moist oxygen. The density of the charged particles was of the order of 1015 m⁻³, while the neutral atom density was as high as 2×10^{21} m⁻³. The neutral atoms do not interact aggressively with viscose materials, so they can diffuse deep into non-woven materials where they cause rather uniform functionalization with polar functional groups as well as the removal of any hydrophobic impurities that might be present on the fibre surfaces. The result of such a deep functionalization is a dramatic improvement of the sorption kinetics. Water and saline solution is soaked by plasma-treated materials about 100 × faster than by untreated materials, and the improvement for exudate and blood is up to an order of magnitude.

Plasma nano-science remains a priority of our research due to promising results and the broad range of future application from photovoltaics to biomedicine. We reported on the chemical synthesis of the arrays of silicon oxide nano-dots and their self-organization on the surface via physical processes triggered by surface charges. The method based on chemically active oxygen plasma leads to the rearrangement of nanostructures and eventually to the formation of groups of nano-dots. This behaviour is explained in terms of

the effect of electric field on the kinetics of surface processes. The direct measurements of the electric charges on the surface demonstrate that the charge correlates with the density and arrangement of nano-dots within the array. Extensive numerical simulations support the proposed mechanism and prove the critical role of the electric charges in the self-organization. This simple and environment-friendly self-guided process could be used in the chemical synthesis of large arrays of nano-dots on semiconducting surfaces for a variety of applications in catalysis, energy conversion and storage, photochemistry, environmental, bio-sensing, and several others.

The characterization of surfaces and interfaces, layered structures and nanomaterials requires the application of advanced surface-sensitive analytical techniques. In our department X-ray photoelectron spectroscopy (XPS), secondary-ion mass spectroscopy (ToF-SIMS), Auger electron spectroscopy (AES) and atomic force microscopy (AFM) have been used successfully, both for basic research and the characterization of technological samples. Our research group is recognized worldwide as a leading group in the research field of the depth profiling of thin films and multilayers with a high depth resolution. In this field we continued studying the influences of different distortion effects on depth resolution upon measurements of the elements distribution in thin films and multi-layered structures. We succeeded to improve the existing mixing-roughness-information (MRI) model describing the influence of atomic mixing by ion bombardment, information depth of the analysed species, and the surface and interface roughness of the specimen. We introduced a new description for interface roughness with an asymmetrical function that differs from the Gaussian function used conventionally in analytical work. A comparison between the model and the experimental determination of the depth profiles shows that a realistic non-Gaussian function has to be taken into account if high accuracy in quantification of sputter depth profiles is required. This is of particular importance for analyses of ultra-thin multilayer structures (up to 10 nm), which are frequently involved in advanced applications.

Aminopropylsilanes bonded on silicon substrates promote adhesion between the inorganic material and organic compounds. Aminosilanes are self-assembled molecules since they form a multi-layer structure on a surface over a certain time span after deposition. Such a modified surface can be used in many applications from biological studies to attaching metal nanoparticles, and sensor applications. We performed a systematic characterization of a silicon surface modified by different self-assembled aminopropylsilanes (APS) with the purpose of using them in sensor applications. Single-crystal silicon wafers were modified with aminosilanes having different numbers of bonding sites: 3-aminopropyl-trimethoxysilane (APTMS), 3-aminopropyldiethoxymethylsilane (APRDMS) and 3-aminopropyl-ethoxydimethylsilane (APREMS). We deposited the self-assembled layers from a solution of aminosilanes in toluene under various reaction conditions. The surface composition, the chemical bonding and the surface morphology were determined using XPS, ToF-SIMS, AFM and SEM. Our results show that the reactivity with the Si-oxide layer and the polymerization of aminosilanes depend on the number of possible bonding sites. The APTMS reacted most intensively with the Si-oxide layer; a less intensive reaction was observed for the APRDMS; and the least intensive reaction was observed for the APREMS. For aminosilane molecules with more bonding sites the effect of the polymerization is more intensive, resulting in island formation and a rougher surface. At 25 °C the polymerization is more intensive than at elevated temperatures, which we attribute to a faster deposition of the molecules at higher temperatures.

In collaboration with the company Melamin from Kočevje, Slovenia, we have studied novel materials for thermal insulation panels. Extensive work of minor elements, thanks to a high sensitivity and lateral resolution.

The recently granted EU project "IP4Plasma" also involves a Slovenian industrial partner Tosama and the major goal is the development of functional textiles.



Figure 5: Simulated ad-atom density patterns defining QD movements upon the exposure of Si wafers to oxygen plasma and corresponding AFM images.



Figure 6: ToF-SIMS characterization of Fe-Sm alloy after annealing at 1250 °C allows for the identification of phases as well as the distribution



Figure 7: A melamine-formaldehyde foam sample that is to be encapsulated in vacuum insulation panels.

performed on rigid melamine-formaldehyde (MF) foams clearly showed it is a suitable material, which may substitute currently used organic foams.

All foams used in a standard way in industrial practise contain additives like bromine, which are added due to the required self-extinguishing properties of insulating materials. Such additives have to be abandoned by 2015. Besides the fact that the MF foams are already self-extinguishable since they contain appreciable amounts of nitrogen, they are also distinguished by a higher application temperature (180°C) comparing to the currently applied foams made on the basis of polystyrene or polypropylene. We tested the MF samples as potential candidates for core materials used in vacuum insulation panels. We developed a unique procedure for the evaluation of the thermal conductivity as a function of pressure in the foam, which also allows for long-term monitoring of the outgassing rate. The evacuated MF foams have a low thermal conductivity of about 6 W/K, which is equivalent to organic foams, but due to the extremely low outgassing rates they are even more suitable for vacuum panels.

Our fusion-related EURATOM project is focused on hydrogen-metal interaction, in particular with fusion relevant metals such as beryllium and

tungsten. These two metals will represent the "first wall" (plasma-facing components) of international fusion reactor ITER. Thermal load and ion impact will induce tritium retention in mixed deposits of tungsten and beryllium. Since only little general data about such films exist, the knowledge should be improved so possible mechanisms involved at interaction between these materials and hydrogen were investigated. We studied properties of films containing various amounts of Be and W. Research on the outgassing rate was performed and subsequent hydrogen/deute-rium gas permeation technique at temperatures up to 400 °C was elaborated. The same method has been applied for characterization of duplex membranes (a low-permeable film on a high-permeable substrate) and has been proved as a reliable technique, so a few papers have been published in last years on pure Be and W films. The most outstanding finding was an extremely high capability of nano-structured W film to retain hydrogen, reaching values as high as about 0.1H/W, which had not been expected since bulk tungsten is renowned for its very low hydrogen solubility. Films with various Be/W ratios were deposited at C. Lungu's laboratory at NILPRP, Bucharest, Romania, by the TVA method and thoroughly characterized by SEM and XPS in order to confirm the range of set values for Be/W ratio. A series of precise hydrogen-permeability measurements combined with long-term outgassing-rate measurements were realized. In addition, various experimental techniques were applied for the evaluation of film properties, like SEM, XRD, XPS and AFM.

Some outstanding publications in the past year

- Lazović, S., Puač, N., Spasić, K., Malović, G., Cvelbar, U., Mozetič, M., Petrović, Z.: Plasma properties in a largevolume, cylindrical and asymmetric radio-frequency capacitively coupled industrial-prototype reactor. Journal of Physics D, Applied physics, 2013, vol. 46, no. 7, 075201-1-075201-8
- Peršin, Z., Devetak, M., Drevenšek Olenik, I., Vesel, A., Mozetič, M., Stana-Kleinschek, K.: The study of plasma's modification effects in viscose used as an absorbent for wound-relevant fluids. Carbohydrate polymers, 2013, vol. 97, issue. 1, 143–151
- Levichenko, I., Cvelbar, U., Modic, M., Filipič, G., Zhong, X., Mozetič, M., Ostrikov, K.: Nanoherding: plasmachemical synthesis and electric-charge-driven self-organization of SiO₂ nanodots. The journal of physical chemistry letters, 2013, vol. 4, issue 4, 681–686
- 4. Liu, Y., Jian, W., Wang, J. Y., Hofmann, S., Kovač, J.: Influence of non-Gaussian roughness on sputter depth profiles, Applied Surface Science, 2013, vol. 276, 447–453
- Zajec, B., Nemanič, V., Žumer, M., Porosnicu Corneliu Lungu, C.: Hydrogen permeability through beryllium films and the impact of surface oxides. Journal of Nuclear Materials, 2013, vol. 443, 185–194

Awards and appointments

1. Asst. Prof. Alenka Vesel; Award for the most cited article in the Journal *Dyes and Pigments* in years 2010 and 2011; title of the article: *"Colorimetric properties of reversible thermochromic printing inks"*

Organization of conferences, congresses and meetings

1. 20th International scientific meeting of Vacuum Science and Technology, Jeruzalem, Ljutomersko-Ormoške gorice, 9.–10. 5. 2013

INTERNATIONAL PROJECTS

- 1. Development of a Vacuum Measurement Method with Respect to Vacuum Glazing AGC Glass Europe Dr. Vincenc Nemanič
- 2. 7FP EURATOM; Removal of Deposits by Neutral Oxygen and Nitrogen Atoms 1.4.2.-FU; 3211-08-000102, FU07-CT-2007-00065
- Ministry of Higher Education, Science and Technology Prof. Miran Mozetič 7 TEP - FURATOM-MHEST 1.4 4-FU: Deuterium Interaction K
- 7FP EURATOM-MHEST, 1.4.4-FU; Deuterium Interaction Kinetics with BE, W and Mixtures Relevant to ITER and DEMO Ministry of Education, Science and Sport
- Dr. Vincenc Nemanič 4. EFDA-JET 2013 Experimental Campaigns
- EFDA-JET 2015 Experimental Campaigns Ministry of Education, Science and Sport Dr. Aleksander Drenik
- 7FP EURATOM-MHEST, WP13-IPH-A01-P3-02/MESCS/PS, Permeation Measurements of Mixed Be/W Layers Ministry of Education Science and Sport
 - Ministry of Education, Science and Sport Dr. Vincenc Nemanič
- EFDA-JET 2013 Analysis of Mixed Materials on ITER-like Wall Samples Using XPS/AES Ministry of Education, Science and Sport Dr. Vincenc Nemanič
- COST MP1101; Biomedical Applications of Atmospheric Pressure Plasma Technology COST Office
- Prof. Uroš Cvelbar
- NATO Planning Grant; SfP 984555; Atmospheric Pressure Plasma Jet for Neutralisation of CBW (Chemical Biological Weapons) NATO - North Atlantic Treaty Organisation Prof. Uroš Cvelbar
- COST TD1208; Electrical Discharges with Liquids for Future Applications; COST Training School on Liquid Discharges COST Office
 - Prof. Uroš Cvelbar
- 10. Plasma Synthesis and Application of Nanowalls Slovenian Research Agency Prof. Uroš Cvelbar
- Plasma Synthesis and Deposition of Quantum Dots Slovenian Research Agency Prof. Uroš Cvelbar
- Determination of Interdiffusion Coefficients in Nano-layered Structures by High Resolution Depth Profiling Slovenian Research Agency
- Asst. Prof. Janez Kovač 13. Plasma Treatment of Titanium Stents Slovenian Research Agency
- Prof. Uroš Cvelbar 14. Plasma-assisted Synthesis of Nano-objects Slovenian Research Agency
- Prof. Uroš Cvelbar
- Formation of Nanocomposite Thin Films in Dusty Magnetized Plasma Slovenian Research Agency Asst. Prof. Alenka Vesel
- Hydrogen Interaction With W/Be Films Relevant for Fusion Reactors Slovenian Research Agency Dr. Vincenc Nemanič
- Characterization of Non-equilibrium Plasma for Modification of Nano and Biocompatible Materials Slovenian Research Agency
- Prof. Miran Mozetič
- Ultra Nanoporous Nanowires of Metal Oxides Slovenian Research Agency Prof. Uroš Cvelbar
- Development and Investigation of Optimal Regimes of RF Conditioning of Uragan-2M Vacuum Chamber Walls using Optical and Probe Methods of Plasma Diagnostics Slovenian Research Agency Prof. Miran Mozetič
- Characterization of Processing Plasma with Catalytic and Cutoff Probes Slovenian Research Agency Prof. Miran Mozetič

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

- Near-Net Shape Nanoparticle-Reinforced Polymer-Composites for Highly-Loaded Advanced Mechanical Components with Superior Tribological Performance Asst. Prof. Janez Kovač
- 2. Organic-Inorganic Thin Film Structures for Electronics Components Asst. Prof. Janez Kovač
- Research and Development of Integrated Overvoltage Protection Devices Based on Gaseous Discharger Toward a Reliable Miniature Technical Solution Dr. Vincenc Nemanič
- Development of Advanced Processes for Attending High Efficient Nano Modified Textile Materials Prof. Miran Mozetič
- Development of the Functional Textiles Used fot the Treatment of Diabetic Foot (Malum perforans)
- Prof. Miran Mozetič6. New Materials for Printed Sensors and Indicators and their Integration in Smart Printed Matter
- Asst. Prof. Alenka Vesel 7. Multifunctional Nanostructured Films for Artificial Implants - Corrosion and Tribocorrosion Processes
- Asst. Prof. Janez Kovač 8. Synthesis of Nanowires for Regenerative Energy Cells
- Prof. Uroš Cvelbar
- Colour, Absorption and Protective Nanolayer Coatings for Aluminium Alloy Asst. Prof. Janez Kovač
- Functionalization of Biomedical Samples by Thermodynamic Non-equilibrium Gaseous Plasma Prof. Miran Mozetič
- Toward Ecologically Benign Alternative for Cleaning of Delicate Biomedical Instruments
- Asst. Prof. Alenka Vesel 12. Self-lubricating and Wear Resistant PVD Hard Coatings Based on (V,Cr,Al,Ti)N for Hotworking Processes Dr. Peter Panjan
- Preparation of Hemocompatible Polymeric Surfaces for Biomedical Applications Dr. Ita Junkar

NEW CONTRACTS

- Investigation of Melamine Foams as the Core Material in Vacuum Thermal Insulation Melamin Chemical Factory, d. d. Dr. Vincenc Nemanič
- Investigation of Evaluation Methods for Vacuum Insulation Panel Performance Testing in Accordance with Draft of ISO Standard
 - Stirolab, d. o. o. Dr. Vincenc Nemanič
- Environmentally Friendly Cleaning of Components for Large Vacuum Systems Vacutech Vacuum Technologies and Systems, d. o. o.
- Prof. Miran Mozetič 4. Characteristics of Gaseous Plasma in Gaps Kolektor Sikom d. o. o.
- Prof. Uroš Cvelbar 5 Advanced Functional Imp
- Advanced Functional Implant Ekliptik, d. o. o.
- EKIIPTIK, d. o. o. Dr. Ita Junkar
- Nanowire Synthesis for Regenerative Energy Cells Kolektor Group, d. o. o.
 - Prof. Uroš Cvelbar
- 7. Functionalization of biomedical samples with thermodynamically non-equilibrium gaseous plasma
- Bia Separations Prof. Miran Mozetič
- 8. Toward Ecologically Benign Alternative for Cleaning of Delicate Biomedical Instruments
- Eliptik, d.o.o. Asst. Prof. Alenka Vesel

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DEPARTMENT OF SOLID STATE PHYSICS

F-5

Our research program is focused on studying 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 behavior of these systems, which represent the link between perfectly ordered crystals, on one side, and amorphous matter, soft condensed matter and living systems, on the other. Such knowledge provides the key to our understanding of the macroscopic properties of these systems and is an important condition for the discovery and development of new multifunctional materials, nanomaterials and biomaterials for new applications. An important part of the research program is devoted to the development of new experimental methods and techniques in the field of magnetic resonance, magnetic resonance imaging, fluorescence microspectroscopy, scanning tunneling, 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 T₁ via field cycling,
- Nuclear double resonance and quadrupole double resonance such as ¹⁷O-H and ¹⁴N-H,
- Fast field cycling NMR relaxometry,
- Frequency-dependent electron paramagnetic resonance (EPR) and 1D and 2D pulsed EPR and relaxation
- MR imaging and micro-imaging
- Measurement of the electronic transport properties
- Magnetic measurements.
- Fluorescence microscopy and microspectroscopy
- Linear and non-linear dielectric spectroscopy in the range 10⁻² Hz to 10⁹ Hz,
- Electron microscopy and scanning tunnelling microscopy,
- Atomic force microscopy and force spectroscopy,
- Dynamic specific-heat measurements.

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

- Magnetic Resonance and Dielectric Spectroscopy of Smart New Materials
- Physics of Soft Matter, Surfaces and Nanostructures
- Experimental Biophysics of Complex Systems

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

The research of the programme group has focused on a study of the physical phenomena in condensed matter at the atomic and molecular levels. The purpose of the investigations was to discover the basic laws of physics governing the behaviour of the investigated systems. The attained knowledge provides the key to the understanding of microscopic and macroscopic properties of various types of solids and is an important condition The group has investigated important open issues in the electronic properties of quasicrystals and complex metallic alloys, quantum magnetism in low-dimensional spin systems, the physical properties of nanostructures, materials with a giant electrocaloric and thermomechanical effect, and multiferroic and relaxor phases. The research included pharmaceutical and biological substances, where a nuclear quadrupole resonance-based technique for the detection of nitrogen complexes (as found in explosives, drugs and narcotics) was developed.

Prof. Igor Muševič





Figure 1: Structure of the TGBA phase and trapping of nanoparticles within the cores of defect lines, thus helping to stabilize the screw dislocations.



Figure 2: Motif from the crystal structure of the cubic metallic phase V-Al₅Cu₆Mg₂



Figure 3: Determination of the magneticanisotropy parameters of the quantum kagome antiferromagnet BaCu3V208(0H)2 in the case of (a) crystal-field anisotropy and (b) Dzyaloshinsky-Moriya anisotropy.

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

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

Using direct measurements it was shown that the maximum electrocaloric response is achieved at the ferroelectric phase-transition temperature. Field-dependent piezoelectric measurements have demonstrated in BaTiO₃ that the field-induced critical point influences the strength of the electromechanical response and the electrocaloric responsivity, both of which exhibit a maximum in the vicinity of the critical point. Using calorimetric and optical experiments we showed that the anisotropic graphene and MoS₂ nanoparticles stabilize the first blue phase in contrast to spherical nanoparticles, which mainly stabilize the third blue phase. Moreover, CdSe spherical quantum dots stabilize the TGB_A phase (see Figure 1), which is an analogue of the Shubnikov phase of type-II superconductors. The above results have been published in 14 articles in international scientific journals. Recently published works on electrocalorics and the stabilization of blue phases have been cited more than 100 times in 2013 alone.

Complex metallic alloys

Combining the measurements of bulk transport properties, specific heat and nuclear magnetic resonance, the group of Janez Dolinšek studied the influence of structural complexity on the physical properties of the cubic intermetallic phase V-Al₅Cu₆Mg₂. With 39 atoms in a unit cell, V-Al₅Cu₆Mg₂ is an intermetallic phase with an intermediate structural complexity (Figure 2). We found that the free-electron approximation provides a good description of the V-Al₅Cu₆Mg₂ behaviour, despite the presence of the quenched structural disorder at low temperatures, which is very likely intrinsic to the structure of V-Al₅Cu₆Mg₂. The work was published in M. Klanjšek, S. Jazbec, M. Feuerbacher, J. Dolinšek, "Physical properties of the V-Al₅Cu₆Mg₂ complex intermetallic phase", *Intermetallics* 39, 50 (2013).

Quantum magnetism

By means of neutron scattering and specific heat measurements, Martin Klanjšek, with French colleagues, studied the magnetic ordering of the quasi-one-dimensional antiferromagnet $BaCo_2V_2O_8$ at low temperatures in magnetic fields up to 12 T. They confirmed the theoretically predicted incommensurate magnetic ordering in fields above 3.9 T and showed that two types of magnetic domains with equal populations develop in the material. They determined the critical exponents for the transitions into the Neél and incommensurate magnetic ordered state. The work was published in E. Canévet, B. Grenier, M. Klanjšek et al., "Field-induced magnetic behavior in quasi-one-dimensional Ising-like antiferromagnet $BaCo_2V_2O_8$: a detailed single-crystal neutron diffraction study", *Phys. Rev. B* 87, 054408 (2013).

By means of ¹³³Cs nuclear magnetic resonance and electron paramagnetic resonance, Denis Arčon, Kristijan Anderle and Martin Klanjšek, with German colleagues, studied the coupling between the electron, lattice, orbital and spin degrees of freedom in the p-electron compound Cs_4O_6 . They realized that the temperature evolution of the measured spectra depends dramatically on the thermal history of the sample. The compound exhibits two competing low-temperature phases, the quenched cubic phase and the low-symmetry phase, where the portion of each phase depends on the cooling protocol. This interesting result is a consequence of the slow reorientation of the p orbitals on cooling. The work was published in D. Arčon, K. Anderle, M. Klanjšek et al., "Influence of O_2 molecular orientations on p-orbital ordering and exchange pathways in Cs_4O_6 ", *Phys. Rev. B* 88, 224409 (2013).

Matej Pregelj, Andrej Zorko and coworkers studied the origin of the magnetic anisotropy in the ${Cu_4(tetrenH_5)[W(CN)_8]_4\cdot 7.2H_2O)}_n$ system. Their results revealed that two-dimensional magnetic correlations start to develop already at 70 K, i.e., well above the magnetic ordering transition. Their modelling of the experimental results shows that the key to the anisotropic response lies within the combination of the dipolar interaction and the axial local anisotropy of the W and Cu ions. Their results were published in O. Zaharko *et al.*, "Source of magnetic anisotropy in quasi-two-dimensional XY ${Cu_4(tetrenH_5)[W(CN)_8]_4\cdot 7.2H_2O)}_n$ ", *Phys. Rev. B* 87, 024406 (2013).

Andrej Zorko, Matej Pregelj, Anton Potočnik, Denis Arčon and collaborators determined the magnetic structure in the ground state of the spin-chain system CuSe₂O₅. This is characterized by

staggered moments with significantly reduced size, as a consequence of quantum fluctuations. By employing various complementary experimental techniques we also determined the magnetic anisotropy of the system, which is responsible for the staggering of the moment as well as for a relatively small critical field, leading to a spin-flop magnetic transition. Their results were published in M. Herak *et al.*, "Magnetic order and low-energy excitations in the quasi-one-dimensional antiferromagnet CuSe₂O₅ with staggered fields", *Phys. Rev. B* 87, 104413 (2013).

Utilizing electron spin resonance, Andrej Zorko and collaborators determined the magnetic anisotropy of the quantum kagome antiferromagnet $BaCu_3V_2O_8(OH)_2$ and showed that this is of the Dzyaloshinsky-Moriya type (Figure 3). They demonstrated that its dominant component is perpendicular to the kagome planes, which significantly suppressed the quantum fluctuations in this system. Freezing of the fluctuations is responsible for the unexpected long-range magnetic ordering of this system at relatively high temperatures, comparable to the exchange interactions. Their results were published in A. Zorko *et al.*, "Dzyaloshinsky-Moriya interaction in vesignieite: a route to freezing in a quantum kagome antiferromagnet", *Phys. Rev. B* 88, 144419 (2013).

Multiferroics

Matej Pregelj, Peter Jeglič, Andrej Zorko, Tomaž Apih, Anton Gradišek, Denis Arčon and coworkers studied magnetically ordered states and the accompanying structural changes in the multiferroic FeTe₂O₅Br (Figure 4). Employing a combination of neutron diffraction and nuclear quadrupolar resonance (NQR) they managed to determine the incommensurate magnetic ordering in the paraelectric state (HT-IC), which exists in a narrow temperature range – just a few Kelvins before the multiferroic state (LT-IC) with finite electric polarization. In addition, they confirmed that electric polarization stems from the magnetostriction of Fe-O-Te-O-Fe exchange pathways, which is related to the phase shifts of the neighbouring magnetic modulation waves. Their results were published in M. Pregelj *et al.*, "Evolution of magnetic and crystal structures in the multiferroic FeTe₂O₅Br", *Phys. Rev. B* 87, 144408 (2013).

As a continuation of the work on the $FeTe_2O_5X$, X = Br, Cl system, Matej Pregelj, Andrej Zorko, Peter Jeglič, Zdravko Kutnjak, Simon Jazbec and Denis Arčon with coworkers studied the magnetic, structural and dielectric properties of the FeTe_2O_5Cl compound. They have discovered that its ground state is multiferroic and that the corresponding magnetic ordering is very similar to the one in the isostructural FeTe_2O_5Br system (Figure 5). They also learned that the main difference between the two isostructural compounds is in the structural effects, accompanying the establishment of the multiferroic phase, which are much more pronounced in FeTe_2O_5Cl. Moreover, they assigned these structural changes to the shift of the O₁ ion and correlated them with the polarization of the Te⁴⁺ lone-pair electrons. In this way they confirmed that the lone-pair electrons are indeed the carriers of the electric polarization in these systems. Their results were published in M. Pregelj *et al.*, "Multiferroicity in the geometrically frustrated FeTe_3O_5Cl", *Phys. Rev. B* 88, 224421 (2013).

Clathrates

In collaboration with Prof. Tanigaki from Japan, Denis Arčon, Andrej Zorko and Peter Jeglič studied type-I germanium clathrates – cage structures with promising thermoelectric properties. Their NMR results are in agreement with claims that the conventional picture of purely ionic interactions between the rattling guest atoms and the cage is only approximate and that covalent

effects should be taken into account in the clathrates or similar thermoelectric cage materials. Their results were published in A. Arčon *et al.*, "Rattler site selectivity and covalency effects in type-I clathrates", *J. Phys. Soc. Jpn.* 82, 014703 (2013).

Studies of crystal structures

Matej Pregelj and coworkers studied copper and zinc complexes with the condensation derivative of 2-acetylpyridine and hydrolyzed ethyl hydrazinoacetate. They determined the crystal structure and discovered that the fifth coordination site of the ligand (Zn/Cu) is occupied by a chloride, causing a distortion of the zinc surrounding. In addition, they studied thermal behaviour employing thermogravimetric analysis. Their results were published in N. Filipović *et al.*, "Synthesis, characterization, and thermal behavior of Cu(II) and Zn(II) complexes with (E)-2-[N-(1-pyridin-2-yl-ethylidene)hydrazino]acetic acid (aphaOH), Crystal structure of $[Zn_2(aphaO)_2Cl_2]$ ", *J. Coord. Chem.* 66, 1549 (2013).



Figure 4: The ⁸¹Br NQR spectra for (a) Br1 and (b) for both isotopes of Br_2 in the high-temperature (HT-IC) and the low-temperature (LT-IC) phases. Thick black lines are simulations considering the magnetic structures determined by neutron diffraction and the derived hyperfine coupling tensors. For a comparison we show simulations of the HT-IC spectra based on the LT-IC structure with an appropriately reduced size of the magnetic moments (thick magenta line).



Figure 5: Magnetic structure models for $FeTe_2O_3X$ (X = Br,Cl), compared at Fe_{11} and Fe_{21} sites for the low-temperature phase in the (a) ab and (b) ac projections, and for the high-temperature phase in the (c) ab and (d) ac projections. For clarity, the magnetic unit cell along b is flattened and the sizes of the magnetic moments in (c) and (d) are magnified by a factor of 3.



Figure 6: Contributions of various dynamic processes to the total proton relaxation as a function of temperature and magnetic field.



Figure 7: A) Sensor responses and error bars to 100 ppm of CO and 100 ppm of H_2 as a function of the operating temperature; B) TEM image of WO₃ nanostructure functionalized with Au nanoparticles. Inset on the bottom left side shows the size distribution of the Au nanoparticles. Label L stands for WO₃ nanostructures, while labels Pt/W, Au/W in Pt/Au/W denote nanostructures decorated with Pt, Au and Pt/Au nanoparticles.

Zeolites

In collaboration with Prof. Igarashi and Prof. Nakano from Japan, Peter Jeglič and Denis Arčon studied alkali-doped zeolites. Zeolites are nanoporous materials with periodic nanospaces (known as cages), which can accommodate a large amount of alkali atoms. For low-doping levels with sodium atoms the low-silica X zeolites are insulating, whereas they become metallic for high-doping levels. The confined geometry of the alkali-metal nanoclusters imposed by the framework cages make enhanced coupling between the electronic and lattice degrees of freedom leading to the formation of polaron states. The ²³Na and ²⁷Al nuclear magnetic resonance (NMR) investigation of low-silica X zeolites suggests strong electron-phonon coupling in support of the proposed polaron model. This work is described in the paper M. Igarashi, T. Nakano, P. T. Thi, Y. Nozue, A. Goto, K. Hashi, S. Ohki, T. Shimizu, A. Krajnc, P. Jeglič and D. Arčon, "NMR study of thermally activated paramagnetism in metallic low-silica X zeolite filled with sodium atoms", *Phys. Rev. B* 87, 075138 (2013).

Molecular dynamics in a blue phase liquid crystal: a 1H fast field-cycling NMR relaxometry study

Liquid crystals exhibiting blue phases are attractive systems to study due to their highly interesting properties in the fields of optics and photonics. We investigated molecular dynamics in a chiral system, called 10BBL, that exhibits blue phase (BP), two twisted grain-boundary phases (TGB), and a smectic C (SmC*) phase. All these phases are stable over large temperature ranges. By means of fast field-cycling NMR relaxometry, we measured the temperature and field dependencies of proton spin-lattice relaxation times. Using theoretical models for different dynamic processes, we determined correlation times, activation energies, etc. for these processes, which include molecular rotations/reorientations, order director fluctuations, layer undulations, self-diffusion, and rotations mediated by translational diffusion along the helical axis (Figure 6). This is the first relaxometric study of a blue phase liquid crystal, published by Anton Gradišek, Tomaž Apih, Valentina Domenici, Vladimira Novotna, Pedro J. Sebastião, in Soft Matter, 2013,9, 10746-10753.

NMR study of molecular dynamics in complex metal borohydride LiZn2(BH4)5

Lithium zinc borohydride LiZn₂(BH₄)₅ (LZBH) was investigated as a potentially interesting hydrogen-storage material due to its high hydrogen content and low decomposition temperature. LZBH shows a structure of two identical interpenetrated three-dimensional frameworks with no bonds between them, which is a unique feature in complex metal hydrides. To better understand the relations between the structure and the thermodynamics of the system, we studied molecular dynamics in LZBH by means of ¹H and ⁷Li NMR spectra and spin-lattice relaxation measurements. Different thermally activated re-orientational processes of BH₄ tetrahedra about their 2-fold and 3-fold symmetry axes were identified from the temperature-dependent proton and lithium spin-lattice relaxation rates and were quantified by their activation energies. Due to the structure, there are two different types of BH₄ tetrahedra; one type is located between two Zn atoms and the other type between one Li and one Zn atom. Our study presents a physical insight into the dynamic properties of LZBH on the microscopic level of atomic groups, providing a link between the microscopic and the bulk properties of this phase. Published by Anton Gradišek, Dorthe B. Ravnsbæk, Stanislav Vrtnik, Andraž Kocjan, Janez Lužnik, Tomaž Apih, Torben R. Jensen, Alexander V. Skripov, Janez Dolinšek, in J. Phys. Chem. C, 2013, 117, 21139–2147.

Nanomaterials

Tungsten oxide nanostructures functionalized with gold or platinum NPs were synthesized and integrated, using a single-step method via aerosol-assisted chemical vapour deposition, onto micro-electromechanical system (MEMS)-based gas-sensor platforms. This co-deposition method is demonstrated to be an effective route to incorporate metal NPs or combinations of metal NPs into nanostructured materials, resulting in an attractive way of tuning the functionality in metal oxides. The results show variations in the electronic and sensing properties of tungsten oxide according to the metal NPs introduced, which are used to discriminate effectively analytes (C_2H_5OH , H_2 , and CO) that are present in proton-exchange fuel cells. Improved sensing characteristics, in particular to H_2 , are observed at 250 °C with Pt-functionalized tungsten oxide films, whereas non-functionalized tungsten oxide films show responses to low concentrations of CO at low temperatures. This work was published in several articles by Polona Umek et al., among others in *Advanced Functional Materials* 23, 1313-1322 (2013).

Substituted imidazole and benzimidazole often form polar hydrogen-bonded chains in the solid state. 2-Methylbenzimidazole is known to be a high-temperature organic ferroelectric. We have measured the temperature dependences of ¹⁴N nuclear quadrupole resonance (NQR) frequencies and proton T_1 in 2-methylbenzimidazole and 5,6-dimethylbenzimidazole. The NQR frequencies are assigned to amino and imino nitrogen positions. The NQR data exclude the possibility of proton two-site exchange in an N–H…N hydrogen bond. The activation energies for the methyl group hindered rotation are determined in both compounds. The present ¹⁴N NQR data are compared to the published ¹⁴N NQR data in solid-substituted and coordinated imidazoles, in substituted benzimidazoles and in imidazole in the gas phase. A linear correlation between the two in-plane principal values of the quadrupole coupling tensor and the out-of-plane principal value of the quadrupole coupling tensor is observed in imidazole, ranging from the amino nitrogen position to the imino nitrogen position. The transition from the amino to the imino nitrogen position is determined on the correlation diagram. The correlation diagram can be used to quantitatively observe the asymmetry of the N–H…N hydrogen bond. A similar correlation diagram is also proposed for substituted benzimidazoles. The magnitudes of the principal values of the ¹⁴N quadrupole coupling tensor in ferroelectric 2-methylbenzimidazole show that the macroscopic ferroelectric ordering has, in this compound, a minor effect on the asymmetry of the N–H…N hydrogen bonds.

Pharmaceutical and biological substances

¹⁴N nuclear quadrupole resonance frequencies have been measured in solid 2-pyridone, 3-hydroxypyridine, and 4-pyridone by ¹H-¹⁴N nuclear quadrupole double resonance. Two slightly non-equivalent nitrogen positions are observed in solid 3-hydroxypyridine, whereas only one nitrogen position has been observed in 2-pyridone and 4-pyridone within the experimental resolution. The rather low ¹⁴N quadrupole coupling constants in pyridones are the consequence of the delocalization of the nitrogen lone-pair electrons in the aromatic rings. Two different compounds have been obtained by the crystallization of 4-pyridone from ethanol in a normal and in a dry atmosphere. The compound obtained in the dry atmosphere is identical to the commercial sample. The compound obtained in the normal atmosphere cannot be converted to the commercial polymorph by melting. It is thus not a polymorph of anhydrous 4-pyridone. The temperature coefficient of the ¹⁴N quadrupole coupling constant is negative in 3-hydroxypyridine and positive in 2- and 4-pyridone. Therefore, in 3-hydroxypyridine, molecular librations dominate the temperature variation of the quadrupole coupling constant, whereas in 2- and 4-pyridone, the changes in the hydrogen bonding interactions with temperature seem to give the dominant effect.

Co-crystals and crystal polymorphs

The 14N and 17O nuclear quadrupole resonance frequencies have been measured in 1:1 co-crystals and salts of 2-amino-4,6-dimethylpyrimidine and several carboxylic acids. A systematic decrease in the ¹⁷O quadrupole coupling constant with the increasing strength of the hydrogen bond is observed in co-crystals bound by O-H...N hydrogen bonds. The O-H distances deduced from the line widths of the ¹⁷O NOR lines show that the hydrogen atom is in a hydrogen bond formed by a carboxylic groups for about 0.01 nm displaced from the oxygen atom toward the centre of the hydrogen bond. In the O-H...N hydrogen bond formed by the hydroxyl group, which is only slightly longer than the hydrogen bonds formed by the carboxyl group, the hydrogen atom is much less displaced. A linear relation between the ¹⁴N quadrupole coupling constant and the sum of the inverse third powers of the H…A (A = O or N) distances is deduced for the amino group. A linear correlation of the principal values of the ¹⁴N quadrupole coupling tensor in NH,, as observed in the solid phase and in the gas phase, is analysed in a simple model assuming a displacement of the electron charge in the N-H σ bond and simultaneous deformation of the nitrogen lone-pair electron orbital. At the ring nitrogen position, hydrogen bonding and proton transfer produce a large decrease in the ¹⁴N quadrupole coupling constant. A linear correlation of the principal values of the ¹⁴N quadrupole coupling tensor is observed in co-crystals and salts of 2-amino-4,6-dimethylpyrimidine. This correlation differs from the correlation observed in substituted pyrimidine, where the hydrogen atoms are replaced by other atoms or functional groups. The difference is analysed in a model, which assumes that the hydrogen bonding and substituents affect the nitrogen lone pair and $\overline{\omega}$ electron orbitals. The analysis shows that the two effects are nearly independent. The application of ¹⁴N NQR to the study of co-crystals and crystal polymorphs is reviewed. In ferroelectric and antiferroelectric organic co-crystals ¹⁴N NQR is used to determine the proton position in an N-H... O hydrogen bond and the proton displacement below T_c. In co-crystal isonicitinamide - oxalic acid (2:1) ¹⁴N NQR is used to distinguish between the two polymorphs and to determine the type of the hydrogen bond (N-...H-O). The difference in the ¹⁴N NQR spectra of the co-crystal formers and the co-crystal is investigated in the case of carbamazepine, saccharin and carbamazepine-saccharin (1:1). The experimental resolution allows an unambiguous distinction between the ¹⁴N NQR spectrum of the co-crystal and the ¹⁴N NQRspectra of the co-crystal formers. The possibility of the application of NQR and the double resonance for the determination of the inhomogeneity of the sample and for the study of the lifetime of an unstable polymorph is discussed.

Amorphous solids

Nuclear quadrupole double resonance (NQDR) is proposed as a method for the quantitative observation of crystallization of amorphous solids. NQDR signals from amorphous and crystalline parts of a sample may be separated. The intensity I of the NQDR signal from the crystalline part of the sample is proportional to its mass. With increasing time the amorphous phase in the sample transforms to the crystal phase and the intensity I approaches its limiting value I_0 , corresponding to a complete transformation to the crystal phase. The ratio I/I_0 is equal to the mass fraction of the crystalline part of the sample. The same experimental method can be used to determine the mass fraction of a given crystal polymorph in a mixture of crystal polymorphs. As an example we studied the crystallization of amorphous nifedipine at 100 °C. The results of the NQDR study are compared to the published results of other studies.

Impact of structure modifications on electrically induced properties of relaxor polymers In collaboration with researchers from Pennsylvania State University, USA, we have investigated how the di-



Figure 8: The nonlinear dielectric response revealed the coexistence of ferroelectric and relaxor states in P(VDF-TrFE) copolymer, irradiated with low doses of high-energy electrons, which was a key point for the explanation of their enhanced electrocaloric response.

electric, electromechanical, and electrocaloric properties of ferroelectric and relaxor polymers (systems that exhibit fast response speeds, giant electrostriction, high electric energy density, and large electrocaloric effect) are affected by various processing procedures and/or modifications, such as (i) stretching the relaxor polymer, (ii) irradiating the ferroelectric polymer with high-energy electrons, and (iii) blending a relaxor polymer with the ferroelectric system. We have recently focused on the P(VDF-TrFE) copolymer that is irradiated with low and moderate doses of high-energy electrons - up to now most of investigations have focused either on ferroelectric P(VDF-TrFE) copolymer or P(VDF-TrFE) that is irradiated with high doses and is thus completely transformed into a relaxor system. Using various experimental techniques we found clear evidence that in such a case ferroelectric and relaxor states coexist in the system, which was a key point for the explanation of their enhanced electrocaloric response. Particularly for the nonlinear dielectric spectroscopy (Figure 8) - we have in fact conducted the first measurements of the real and imaginary parts of the nonlinear dielectric response in ferroelectric and relaxor polymers - was found as an extremely powerful tool for investigating the correlation between the structure and the property evolution in relaxor polymer systems. Published in: G. Casar, X. Li, J. Koruza, Q. M. Zhang, V. Bobnar. Electrical and thermal properties of vinylidene fluoride-trifluoroethylene-based polymer system with coexisting ferroelectric and relaxor states. J. Mater. Sci. 48, 7920 (2013).

High-temperature dielectric investigations of a novel inorganic relaxor system

We have continued high-temperature dielectric investigations of classical inorganic relaxors, which revealed astonishing results - they contradict widely the accepted dogmas on relaxor properties. Also the results obtained in a novel $Pb(Sc_{1,0}N_{1/2})O_{2}$ ceramic system, prepared from mechanochemically activated powder, clearly reveal that



Figure 9: The decay of echo amplitudes during the SLSE experiment with rectangular pulses and QCPMG experiment with WURST pulses. For comparison also the T2 decay is shown. The sensitivity of each experiment is here roughly proportional to the area below the curves. Published in: A. Gregorovič, T. Apih, J. Mag. Res. 233, 96 (2013).

 ${}_{2}N_{1/2})O_{3}$ ceramic system, prepared from mechanochemically activated powder, clearly reveal that the polar nanoregions do not form at the so-called Burns temperature (approx. 600 K), but are continuously formed over a broad temperature range, starting well above 800 K. We have in fact successfully recognized various distinctive dielectric contributions in a broad temperature range of 150–750 K. Moreover, a detailed analysis of the intrinsic high-temperature dielectric response revealed a critical behaviour associated with universality classes typically found in spin glasses and, particularly, that the low-temperature fingerprint behaviour can be observed at much higher temperatures, well above the dispersive relaxor dielectric maximum.

Published in: V. Bobnar, H. Uršič, G. Casar, S. Drnovšek. Distinctive contributions to dielectric response of relaxor ferroelectric lead scandium niobate ceramic system. Phys. Status Solidi B 250, 2232 (2013).

"WURST-QCPMG sequence and "spin-lock" in 14-N Nuclear Quadrupole Resonance"

The excitation of magnetization in Nuclear Quadrupole Resonance (NQR) is most often accomplished with the use of rectangular RF pulses, where the pulse amplitude and phase are constant during the pulse. These pulses are technically easy to implement. Also, they are easy to include in various theoretical predictions and analysis. However, rectangular pulses also have some disadvantages. When these disadvantages become severe, shaped pulses are often used instead. Here, the amplitude and phase during the pulse follow a prescribed function. WURST pulses are

just one of the many shaped pulses and are in use in NMR for a decade. Their principal advantage is a large excitation bandwidth at low RF powers. In the publication we demonstrate that WURST pulses are suitable for 14-N NQR as well. In particular, we demonstrate, that the "spin-lock" effect is completely preserved compared to rectangular pulses. This is very important, as the spin-lock effect is essential for the 14-N NQR detection. It allows us to increase the otherwise poor sensitivity by 10-100 times (Figure 9). The theoretical prediction/analysis of the spin-lock effect is already challenging for the rectangular pulses. For shaped pulses it would be even more difficult. Thus the existence of the spin-lock effect for WURST pulses is not at all obvious. In the publication we have shown how the WURST pulses combined with the QCPMG sequence can significantly reduce the time required for the acquisition of a very broad 14-N spectrum, usually a very time-consuming task. In addition, WURST pulses require limited RF power, and are as such appropriate for small desktop applications of 14-N NQR.

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

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

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

Highly constrained topological defects in nematics

Topological defects in uniaxial nematics can be compared to the defects in biaxial media. The defects are not equivalent, but similarities can be exploited to better understand the topological rules that govern the disclinations in uniaxial nematics. Disclination lines with variable profiles are systematically described with quaternions, which allow the simple characterization of disclinations by counting geometrically recognizable features (Čopar and Žumer, PRSA 469, 2013). In a similar fashion, the bulk director, away from the defects, can be studied as a biaxial phase by using its derivatives. This formulation finds "quasi-disclinations" that carry additional topological Figure 10: 3D image of a nematic colloidal crystal, information, potentially useful for a description of the blue phases and general chiral nematics reconstructed from fluorescent confocal imaging. (Čopar et al, PRE 87, 2013).

3D nematic colloidal crystals

Significant advancements have been made in our understanding of assembling 3D nematic colloidal crystals. We have published in Nature Communications (Nych et al, Nature Commun. 4, 2013]) an article about the laser-tweezers-assisted assembly of 3D nematic colloidal crystals from dipolar nematic colloids. Using fluorescent confocal microscopy we have found that the unit cell of this 3D crystal is tetragonal with a basis (Figure 10). This crystal shows unusual response to external electric fields; for positive dielectric anisotropy of the nematic liquid crystal, the crystal shrinks up to 30%. If the dielectric anisotropy of the carrier nematic liquid

crystal is negative, then the colloidal crystal rotates as a solid unit. The angle of rotation is up to several tens of degrees.

Nematic colloids

In nematic colloids, advances have been seen in a systematic numerical and theoretical study of disclination networks in the interstitial space of a close-packed lattice of homeotropic particles has revealed a model (Figure 11) that explains the reconfigurable interconnected defects in simplest geometric terms. Local description using tetrahedra and cubes is used to construct all the possible arrangements of defects in this highly frustrated environment (Čopar et al, Soft Matter 9, 2013).

Further pair interactions between colloidal particles in confined cholesteric cells have been measured. The interaction profile contains energy minima and thus allows metastable states, the number of which increases with chirality. A description for this phenomenon has been postulated



Figure 11: Modelling of the disclination network in nematic permeating opal structure.



We have investigated the topology and photonics

of liquid-crystal colloids and dispersions, and

studied the motion of molecular motors. New

nanocomposite materials have been developed,

the structure of matter has been studied on the

atomic level and a new infrastructure for cold

atom physics experiments was set up.



Figure 12: Colloidal pair in an unwound chiral nematic in a bubble-gum structure. a-e visualization of the director fields and ordering tensor derivatives. f simulated polarization microscopy

and probed with computer simulations (Jampani et al, PRL 110, 2013). Related studies of colloidal systems with morphologically and topologically different parameters, performed in collaboration with foreign groups, yielded publications in co-authorship (Gharbi et al, Soft Matter 9, 2013; Geng et al, Soft Matter 9, 2013; Cavallaro et al, Soft Matter 9, 2013; Cavallaro et al, PNAS 110, 2013).

Visualization of nematic defects

Analysis of the data produced by numerical simulations and advanced experimental methods requires a host of visualization methods to highlight the parameters of interest (Figure 12). An expansive review over the most common methods has been published, together with examples based on well-known models (Čopar, Porenta, Žumer, Liq. Cryst. 2013).

Nanoparticles dispersed in mesophases

We have demonstrated experimentally and theoretically that the interaction between nanoparticles and topological defects induces a twist-grain boundary phase in a chiral liquid crystal. The occurrence of this phase, the analogue of the Shubnikov phase in type-II superconductors, is driven by the direct interaction



Figure 13: Impact of curvature on the number and position of topological defects.

between surface-functionalized CdSe quantum dots and screw dislocations. It is shown that, within a universal adaptive-defect-core-targeting mechanism, nanoparticles of the appropriate size and functionalization adapt to qualitatively different cores of topological defects such as disclination lines and screw dislocations. The findings suggest new pathways towards the controlled assembly of superstructures in diverse, symmetry-broken, condensed-matter systems, ranging from nanoparticle-decorated liquid crystals to superconductors (G. Cordoyiannis et al., Soft matter 9, 3956 (2013)). Furthermore, we have studied the impact of surface-functionalized graphene nanosheets on the blue-phase range of a chiral liquid crystal. Calorimetric and optical measurements demonstrate that the resulting soft nanocomposite exhibits an increased blue phase temperature stability range for a minute concentration of dispersed graphene. The impact is stronger on the more ordered, cubic structured blue phase I. Experimental results were discussed in the frame of Landau-de Gennes mesoscopic model in terms of the tensor order parameter. These findings suggest that anisotropic nanoparticles may be of great usefulness for stabilizing the blue phases (M. Lavrič et al., Appl. Phys. Lett. 103, 143116 (2013)).

Membrane budding and formation and release of microvesicles

The latter might play an important role in long distance cell-cell communication owing to their ability to move with body fluids. Several mechanisms exist that might trigger pinching off of globular buds from the parent membrane (vesiculation). We have considered theoretically the impact of topological defects (TDs) on this process in the membranes exhibiting global in-plane orientational order. Landau-de Gennes type theoretical approach is used in terms of the tensor orientational order parameter. We show on membrane structures exhibiting spherical topology that the coexistence of regions with positive and negative Gaussian curvature might trigger pairs *defect*antidefect for strong enough local membrane curvatures. Critical conditions for this event are determined for several demonstrative cases (Figure 13). We claim that concentration of TDs at narrow necks might trigger membrane fission neck rupture, enabling a membrane fission process and the release of membrane daughter microvesicles (D. Jesenek et al., International journal of nanomedicine 8, 677 (2013)).

Photonic properties of smectic fibres

In 2013, a lot of attention was paid to our studies of the photonic properties of liquid crystal dispersions. We



Figure 14: Smectic-A liquid crystal spontaneously forms optical fibres that are excellent waveguides and laser emitters.

have studied the resonant transport of light between a planar polymer waveguide and a nematic droplet-optical microresonator in close proximity to the waveguide. White light from a supercontinuum laser that was guided along the planar waveguide, it was seen to be resonantly transferred via photon tunnelling into the Whispering Gallery Modes of the microresonators. A theoretical analysis was also performed within the coupled-mode approach, the article was published in Jampani et al. Optics Express 2013. In the same journal we published in December 2013 in cooperation with partners from Max Planck Institute, Goettingen, an article on the lasing and waveguiding in smectic-A optical fibres (Peddireddy et al, Optics Express 2013). We observed that in contact with water and CTAB, a smectic liquid crystal spontaneously forms micrometre-diameter fibres. Using confocal microscopy, we reconstructed the layered structure of these fibres. The smectic layers are wrapped-up into a series of closed and concentric molecular layers, forming a +1 topological defect in the core of the fibre. These fibres are excellent waveguides and it is possible to induce laser emission from fibres doped with fluorescent molecules (Figure 14). The article has attracted

considerable attention, because it was selected by the editors of all the Optical Society of America journals as the highlight article of December 2013. We have also published a review article on the photonics and topology of nematic colloids and dispersions (I.Muševič, Phil. Trans. Royal Soc. A 2013).

Molecular motors

We developed a model for the dynamics of cytoplasmic dynein, which is one of the largest and most complex motor proteins. We used an elastomechanical model for each individual dynein head and combined it with a minimal model of the chemical cycle of ATP hydrolysis. We showed that a dimeric molecule, consisting of two heads, can synchronize their cycles and step with regular 8-nm steps if the coupling is sufficiently strong (Figure 15). This is the stepping pattern observed in mammalian dynein. With weaker coupling the heads lose synchrony and move with a much

broader distribution of step sizes, but it is still capable of pulling a load. The mode of stepping then corresponds to that observed in yeast dyneins. This shows that the walking mechanism of dynein is robust in itself, but its efficiency and processivity are improved significantly by the coupling between the heads (A. Šarlah and A. Vilfan, The winch model can explain both coordinated and uncoordinated stepping of cytoplasmic dynei; submitted).

LC applications

The Jožef Stefan Institute (JSI) and its spin-off Company, Balder Ltd that was acquired by the multinational Kimberly Clark Corporation (KC) in 2012 were in the past years intensively developing the new concept of LC optical light shutters based on optically compensated birefringence in Super-twisted LCDs. The innovative technical solutions were upgraded (24.9.2013) with a Continuation-in-part Patent US 8,542,334. The new LC light shutter technology is finally protected by 6 granted international patents (USA and EU). The above technology based on the proprietary IP allows Balder (KC) to become the only producer of the LC welding filters in the world that can label its products with the prestigious CE 1/1/1/1 quality certificate. On the grounds of the high performance of Balder's (KC) products, the International Standard Organization invited JSI to Figure 16: Spatial light filtering glass. participate in the ISO expert group ISO/TC94/SC6/WG2 and WG4 preparing new ISO standard

on Eye Protection. The new LC light-shutter technology was recently (2013) upgraded by the emerging spatial light filtering technique (Figure 16). It allows the extension of the application of the LCD optical filters into the field of light hazard (e.g., glare) eye protection against collimated light sources (e.g. car headlights).

Low-friction nanomaterials

In the paper entitled "Nanoparticles as novel lubricating additives in a green, physically based lubrication technology for DLC coatings", M. Kalin, J. Kogovšek, and M. Remskar, Wear 303, 480 (203), we report on a significant improvement of the friction behaviour of diamond-like carbon (DLC) tribological contacts by addition of MoS₂ nanotubes into PAO oil in 2 wt.%. The friction coefficient measured in the most severe conditions was reduced by up to 50%, compared to using only base PAO oil. In the paper "Influence of surface roughness and running-in on the lubrication of steel surfaces with oil containing MoS, nanotubes in all lubrication regimes", by J. Kogovšek, M. Remškar, A. Mrzel, and M. Kalin, Tribology International 61, 40 (2013), we reported that the friction at the steel contact drops by 40-65% when 2 wt.% of MoS, nanotubes are added to base oil. Furthermore, using MoS, nanotubes, the friction is the same for rough and smooth steel surfaces, which indicates a reduced need for fine surface finishing when surfaces are lubricated by MoS₂ nanotubes.

Nanoelectronics

In the paper "Comparative study of chemically synthesized and exfoliated multilayer MoS2 field-effect transistors ", HS Hwang, M. Remškar, et al., Applied Physics Letters, 102, 043116-1 (2013), we report on field-effect transistor (FET) device based on as-synthesized MoS, nanoflakes in comparison to thin flakes prepared by exfoliation of bulk MoS., The transistor characteristics were found to be almost identical; the on/off current ratio is 10⁵ and transistor behaviour of n-type.

Polymer nanocomposites

In the paper "A novel structure of polyvinylidene fluoride (PVDF) stabilized by MoS, nanotubes", M. Remskar, et al., Soft Matter 9, 8647 (2013) we report on the first polyvinylidene fluoride (PVDF)-MoS, nanotube based nanocomposites. The results indicate that the polymer-nanotube interaction stabilizes a novel 2b stacking within the y-phase, which represents a new PVDF crystal structure. Annealing of the PVDF-MoS2 nanotube films leads to a completely relaxed α -phase with the nanotubes forming the nucleation centres for crystallization of the dendritic phase. Tribological properties of these films, which evidence that 1 wt.% of MoS, nanotubes in PVDF reduces fric-





Figure 15: Stepping of a model cytoplasmic dynein molecule.



Figure 17: High-resolution STM image of a Pb monolayer on a Cu(111) surface, showing a Moire pattern. (size 50 x 50 nm2, It=91 mV, Ut=0.8 nA, T=4.2K).

tion by more than 20% with regard to pure PVDF, while 2 wt.% by more than 70%, were published in the paper "Friction properties of polyvinylidene fluoride with added MoS2 nanotubes", M. Remškar et al., *Physica Status Solidi. A, Applications and Materials Science*, 210, 2314 (2013). Raman spectroscopy revealed that sliding in the boundary lubrication regime can trigger the phase transformation to polar PVDF phase in similar way as the drawing during crystallization.

Nanosafety

We prepared a leaflet entitled "Fireworks and other pyrotechnics for entertainment poison air" with the goal to raise awareness of hazardous air pollution by nanoparticles released during fireworks and the combustion of sparklers. The leaflet is available at the public link http://www. uk.gov.si/fileadmin/uk.gov.si/pageuploads/pdf/Ognjemeti_dokoncna.pdf,

Nanoscale superconductivity

Confined metal nanostructures, such as monolayers or small islands of different thicknesses, are very interesting for probing the ultimate limits of nanoscale superconductivity. We are studying the relationship between bulk and nanostructure superconductive critical temperatures (T_c). In particular, we are trying to control Tc on a nanoscale. High-quality Pb ultra-thin films (from one to few monolayers thick) have been deposited in ultra-high vacuum on an atomically flat Cu (111) surface. For low coverage a monoatomic hexagonal close-packed Pb film is formed, which shows

an inverse corrugation (Figure). For higher coverage, a Stranski–Krastanov growth of 3D Pb islands is observed, several monolayers thick. Low-temperature STM and STS measurements were performed down to 1K on such surfaces to study their atomic and electronic structures.

Charge density wave compounds

The real crystal structure of the (NbSe4)(10/3)I charge density wave (CDW) compound was studied by simulation of the X-ray diffuse scattering. The average structure of the low-temperature twinned phase was determined



Figure 18: Schematic representation of an UHV system, built and tested for experiments with ultracold Cs atoms.

and the phase transition was attributed to the formation of a CDW. In addition to the experiments, the electronic properties of the high- and the low-temperature phases were calculated with the extended Hückel tight-binding method. The Fermi surfaces of the average structures above and below the phase transition appear very similar and their shapes support a nesting instability and a CDW formation.

Ultra-cold atoms

An in-house-built ultra-high vacuum apparatus was constructed and tested for experiments on strongly correlated systems with Cs atoms (Figure). Next, different laser systems are being set up, which will in combination with magnetic fields be used to slow down, capture, compress and cool down atoms to nK temperatures.

III. Research programme "Experimental Biophysics of Complex Systems"

Within the program "Experimental Biophysics of Complex Systems" we explore processes and structures of various complex systems (from model systems to the structures in living cells, tissues and even small animals) including the effects of various bioactive molecules like toxins, drugs, etc., as well as of various materials like nanomaterials and medical materials on these systems. Our research is focused on the investigation of structural properties of different membrane structures such as membrane domains, membrane proteins and glycosaccharide matrix as well as their interactions with various materials that enter into their native environment. Novel spectroscopic and

By the analysis of the polarization dependence of fluorescence, we revealed that some widely used membrane probes undertake several lipid phase-dependent conformations at distances below optical spatial resolution. Based on detailed optical microscopy measurements of the dissolution of blood clots model in an artificial perfusion system, we have developed a mathematical model describing the thrombolysis as a corrosion-erosion process. microspectroscopic techniques contribute to the understanding of the organization of these supramolecular systems, complex cell and tissue responses as well as opening new possibilities to design new medical materials, like scaffolds for tissue regeneration as one of the most relevant problems in the current aging population of the developed countries. In addition, we focus on medical method optimization, like tumour treatment methods, magnetic resonance imaging and the mathematical modelling of trombolisis, magnetic resonance microscopy in forestry, wood science and food processing as well as to restricted diffusion research.

One of the hottest topics of current biophysics is certainly the study of the interactions between novel materials and cells, especially from the
bioactivity and biocompativility point of view, which we explore by applying novel microspectroscopies. The basic questions is: do nanoparticles and nanofibres enter cell membranes. The partitioning of the nanoparticles was studied via FMS-FRET experiments on model membranes, exposed to the diffusing nanoparticles on a micron scale. The nanoparticles first accumulated on membranes coming into the molecular neighbourhood of the membrane probes, which enhanced the membrane probe signal due to FRET. After approximately 40 min. the liposomes start to degrade and the membrane signal was detected everywhere within the micrometre neighbourhood.

Our system for fluorescence microspectroscopy enables us to acquire fluorescence spectra from microscopic volume elements of the sample and thus to detect physical changes in local molecular environment of fluorescent probes. By stochastic wavelength sampling and efficient computer simulations we improved spectral resolution and bleaching correction reliability, as we reported in the published article "Bleaching-corrected fluorescence microspectroscopy with nanometer peak position resolution. Opt. Express vol. 21, no. 21, p. 25291-25306". Upgrading the analysis by polarization dependence of emitted fluorescence, we revealed that some widely used membrane probes undertake several lipid phase-dependent conformations at distances below optical spatial resolution. We published our findings in the article "Coexistence of probe conformations in lipid phases: a polarized fluorescence microspectroscopy study. *Biophys. j.*, vol. 105, no. 4, p. 919-927". As a part of our cell-nanomaterial interaction research, we used resonance energy transfer imaging to investigate rates and mechanisms of titanate nanoparticles' penetration through membranes of giant vesicles. The system for optical micromanipulation was used to study the dynamics and strength of cell attachment to macrostructured biomedical materials that are used as models for potential artificial tissue scaffolds. The results were correlated by molecular (EPR) and macroscopic (morphology, rheology, viscoelasticity) properties of the scaffolds.

In the area of the design and synthesis of probes (nitroxide, fluorophore and combination of both in the same molecule) in 2013 focus was on the synthesis of environment sensitive fluorescent probes (sensitive to polarity and hydration of the environment). A small series o fluorophores was synthesized by linking of 7-(diethylamino) coumarin and different aromatic systems with oxazole. Synthesized dyes display red shift of absorption as well as emission spectra. Fluorescence emission spectra in solvents of increasing polarity exhibit decrease of fluorescence intensity and red shift of emission maxima. Under our experimental conditions synthesized fluorophores display excellent photostability compared to NBD type probes. 7-(diethylamino)coumarin represented also the basis of for a small series of double spin-fluorescent probes. The influence of distance between fluorophore and nitroxide was examined with these probes. Several pH dependant probes of rhodamine type were also evaluated in regard to their photophysical properties.

In collaboration with Biotechnical faculty we have investigated how structural properties of several phenolic substances influence their binding and interaction with liposome membranes. Phenolics are antioxidants with antimicrobial effect and are therefore interesting as bio-additives for food industry. Results obtained using EPR, fluorescence anisotropy and differential scanning calorimetry show that phenolics investigated decrease membrane fluidity and are bounded to a membrane surface predominately via hydrogen bonds (Food chemistry, 2013,139:804-813).

In collaboration with Hacettepe University, from Ankara, Turkey, the influence of tricyclic antidepressant clomipramine (CLO) on model and biological stratum corneum (SC) membrane was investigated by EPR. The fluidizing effect of CLO on pig ear SC throughout the whole membrane indicates that CLO penetrates into the stratum corneum, which is important for its transdermal delivery (J. Pharm. Sci. 2013, DOI 10.1002/jps.23687).

In collaboration with Max Delbrück Center for Molecular medicine in Berlin, Germany, we have investigated the role of lisophospholipid, perifosine (OPP) as a constituent of liposome membrane on trans-cell barrier transport of liposome encapsulated drugs. We have shown that liposome membrane fluidity decreases with increasing concentration of perifosine in liposomes. This could be a reason for the increased release of the liposome encapsulated hydrophilic substance measured with the increasing concentration of perifosine. Our results indicate that the efficient transport of liposome-encapsulated hydrophilic drugs across the barrier into a disease-affected tissue is possible with liposomal formulations, which contain sufficient amounts of perifosine to open the channels in the barrier and release the liposome content when the cell barrier is compromised. This opens a new possibility of using lysolipid-containing liposomal formulations as drug delivery systems (submitted for publication).

We have recently shown that the structure of water confined between lipid membranes is perturbed with respect to bulk water. Due to a low light penetration depth the attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy is specifically suited to study interlamellar water structure in multibilayers. Sequential modification of interlamellar water perturbation can be followed with a step-by-step dehydration of samples either by water evaporation or by osmotic pressure. Besides different levels of hydration, the lipid-water interaction can be studied for lipids with different headgroups and for different lipid phases. Modification of interlamellar water properties could explain water-mediated effects on biological processes. This can have implications to membranes adhesion, stacking, and fusion.

Using molecular dynamics (MD) we calculated partition coefficients between the membrane and water phase for several commonly used labels (two spin labels and a fluorescent marker). Coefficients were obtained by first calculating the free energy for the transition from the membrane into water using adaptive biasing force (ABF) MD. The results allow us to perform experiments with greater precision and more economically. Part of the results is summarized in the graduation work of Klare Presecnik with the title "Determination of partitioning coefficients of amphiphilic molecules between membrane and water using molecular dynamics (ABF)". We have created a generally applicable software package for determining position-dependent diffusion coefficients (available at github.com/lbf-ijs/DiffusiveDynamics). The package is capable of obtaining and visualizing diffusion for one- and two-dimensional cases. With the obtained diffusion surface and a known free energy surface, diffusive trajectories can be generated. Thereby the time reach of molecular dynamics, typically a few 100 nanoseconds, can be extended to several 100 microseconds (for the 1D or 2D subspace of interest). The method for determining the diffusion is most efficiently used with ABF MD. With this methodology, the motion of spin labels in the membrane can be studied, thus further improving the empirical approximation used by side-chain conformational space modelling of proteins (CSM). Such estimates allow us to significantly reduce the computational time needed for determining the size of the side-chain conformational space. This also enables us to solve inverse problems - for example, the structural characterization of membrane proteins.

We started experimental work on cysteine mutants of the N-terminal part of the antimicrobial peptide β -defensin. The ultimate purpose of the experiments is to determine the 3D structure of peptides in various environments using CSM. Using circular dichroism (CD) and the EPR we observed two different conformations we have already observed two conformations. We also discovered conditions under which the transition between conformations can be controlled by varying the pH.

The use of one-dimensional nanoparticles, such as TiO₂ nanotubes, offers a promising low-cost and effective alternative to current disinfection methods used in food processing industry and in hospital environment. In order to improve antibacterial properties of surfaces we developed a stable deposition of TiO₂ nanotubes on polyethylene terephthalate (PET) surface, a material commonly used in food processing industry and hospital environment. PET surfaces with this kind of antibacterial nanocoating (ABnC) retard growth of bacteria by up to one order of magnitude when illuminated by ordinary fluorescent light bulbs.

Thrombolysis is the process in which the addition of specific agents (thrombolytic agents) in the bloodstream can dissolve the blood clots. The usual way that a thrombolytic agent functions is that it initially activates a molecule of plasminogen to its active form plasmin and this in turn degrades the fibrin network of which the clot is made. In a large study, which was started two years ago, we studied the possibility of using a direct thrombolytic agent in which the conversion of plasminogen to plasmin would no longer be needed. Namely, in the bloodstream was directly added plasmin. Its effect on thrombolysis was then followed by an optical microscope, by which we monitored the progress of degradation of artificial blood clots in contact with plasmin molecules. The process of blood clot dissolving was also recorded with a digital camera and images were then analysed so that we could analyse the dynamics of blood clot dissolution. The obtained results were then analysed by an appropriate mathematical model of blood clot dissolution. The findings of this study were published in the journal Blood coagulation and fibrinolysis, another article with similar content is in the publishing process in the Thrombosis Research.

The magnetic resonance imaging (MRI) can also enable monitoring of the development of caries of the teeth and dental tissue impairment caused by caries. However, MRI has of course a number of limitations. The first is that MRI of teeth is currently too demanding that it could be performed *in vivo* successfully. Therefore, our study had to be performed on extracted teeth. Another limitation is that MRI is not capable of imaging of hard dental tissues such as enamel and dentin, at least not in its standard way. However, we still come up with interesting findings with regard to caries. Namely, one of the effects of caries is also dentin demineralization. Due to the demineralization carious dentin produces much more signal than intact dentin, so that regions of demineralized dentin can be easily detected with T1-weighted imaging. Another interesting finding is that caries also affects dental pulp tissue. The changes can be clearly seen in maps of relaxation time T2, as well as in maps of apparent diffusion constants (ADC). The findings of the study were recently published in the Caries Research.

Magnetic resonance imaging allows monitoring of the distribution of electric current density in the conductive samples. By using current images in several different arrangements of electrodes, it is possible to determine the electrical conductivity of the sample and consequently also the electric field for a given electrode arrangement. This is of paramount importance in electroporation, which is a method in which by the use of high voltage cell membrane is a tissue are made temporary permeable and therefore absorb more drugs than normally, as for example anticancer drugs. In this area in the past year, we worked with a group of prof. Damian Miklavčič from the Faculty of Electrical Engineering. Within this collaboration, we conducted a number of important *in vivo* MRI experiments of current distribution during electroporation last year. Until last year these experiments were successfully done only on model samples, but not on experimental animals. Experiments on animals have greater importance because

they can be used for determination of the presence and extent of the region of reversible electroporation. In this region, the tissue cells open for a short time and in this time an anticancer drug can enter the cells, after that the cells close again. Cancer cells in this process die while most of healthy cells should survive. In our experiments, instead of the anticancer drug a MRI contrast agent was injected into experimental animals. In the region of reversible electroporation is the contrast agent remained in the tissue also after several days while it was not present at that time in other tissues that were not reversibly electroporated. Thus, we were able to detect the region of reversible electroporation and also to compare its extent with predations for the region that were done based on calculations of electric field strength on the basis of the measured current density distribution. The findings of this study were sent to the journal Radiology.

Controlled drug-delivery systems are widely used in pharmaceutical industry because of their numerous advantages. For hydrophilic polymers, it is generally accepted that, once in contact with body fluids, they hydrate and swell, forming a gel layer that regulates the penetration of body fluids into the tablet and the dissolution of the incorporated drug. Therefore the knowledge of the gel layer characteristics is of a crucial importance for the use of controlled drug delivery systems. Combination of different MRI methods enables accurate determination of medium penetration into the tablet as well as hydrogel formation *in situ*. MR imaging was used to study the impact of a soluble active substance in the dynamics of the penetration of the medium into the tablet and the formation of the gel layer. Acquired knowledge in this area was found interesting for our pharmaceutical company Krka, for which numerous studies were conducted within the last year.

The method of application of the gradient pulses in combination with the spin-echo (PGSE method) enables measurement of the translational motion. In this method there several free parameters of the PGSE sequence, which may affect how sensitive this method is for detection of the diffusion spectrum. The same method can be adjusted for measurement of the fast motion on a short time scale as well as of the slow motion on the longer time scale, depending on the parameters of the method. These features of the PGSE method were confirmed by measurements on molten polyethylene. The results confirm a model of constraint release in a system of entangled polymer chains as a sort of tube Rouse motion. The results of this research were published in the Journal of Magnetic Resonance.

Our research has been supported by a number of international projects financed by the European Union within the 6th and 7th Frameworks. It was also supported within the bilateral Slovenian – USA, Slovenian – German and Slovenian – Greek and other scientific cooperations. In 2013, the Department had cooperations with 108 partners from Slovenia and abroad. Among them:

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

made the above studies possible.

Some outstanding publications in the past year

- Vallejos, S., Umek, P., Stoycheva, T., Annanouch, F., Llobert, E., Correig, X., de Marco, P., Bittencourt, C., Blackman, C.: Single-step deposition of Au- and Pt-nanoparticle-functionalized tungsten oxide nanoneedles synthesized via aerosol-assisted CVD, and used for fabrication of selective gas microsensor arrays. *Advanced Functional Materials* 23, 1313–1322 (2013)
- Gradišek, A., Bomholdtravnsbaek, D., Vrtnik, S., Kocjan, A., Lužnik, J., Apih, T., Jensen, T., Skripov, A. V., Dolinšek, J.: NMR study of molecular dynamics in complex metal borohydride LiZn₂ BH₄₅. *Journal Phys. Chem. C* 117, 21139–21147 (2013)

- Pregelj, M., Zorko, A., Zaharko, O., Jeglič, P., Kutnjak, Z., Jagličič, Z., Jazbec, S., Luetkens, H., Hillier, A. D., Berger, H., Arčon, D.: Multiferroicity in the geometrically frustrated FeTe₂O₅Cl. *Phys. Rev. B* 88, 224421-1-10 (2013)
- Nych, A., Ognysta, U., Škarabot, M., Ravnik, M., Žumer, S., Muševič, I.: Assembly and control of 3D nematic dipolar colloidal crystals. *Nature Communications* 4, 1489-1-8 (2013), doi: 10.1038/ncomms 2486.2013
- 5. Jampani, V. S. R., Škarabot, M., Čopar, S., Žumer, S., Muševič, I.: Chirality screening and metastable states in chiral nematic colloids. *Phys. Rev. Lett.110*, 177801-1-5 (2013)
- Novak, S., Drobne, D., Vaccari, L., Kiskinova, M. P., Ferraris, P., Birarda, G., Remškar, M., Hočevar, M.: Effect of ingested tungsten oxide (WO_x) nanofibers on digestive gland tissue of Porcellio scaber (Isopoda, Crustacea) : fourier transform infrared (FTIR) imaging. *Env. Sci. & Tech.* 47, 11284–11292 (2013)
- 7. Bajd, F., Serša, I.: Mathematical modeling of blood clot fragmentation during flow-mediated thrombolysis. *Bioph. Journal 104*, 1181-1190(2013).
- 8. Urbančič, I., Ljubetič, A., Arsov, Z., Štrancar, J.: Coexistence of probe conformations in lipid phases : a polarized fluorescence microspectroscopy study. *Bioph. Journal 105*, 919–927 (2013)

Some outstanding publications in 2012

- 1. Guttmann, P., Rembein, S., Bittencourt, C., Umek, P., Ke, Xi., van Tandeloo, G., Ewels, C. P., Schneider, G.: Nanoscale spectroscopy with polarized X-rays by NEXAFS-TXM. *Nature Photonics* 6, 25–29 (2012)
- Dolinšek, J.: Electrical and thermal transport properties of icosahedral and decagonal quasicrystals. *Chem. Soc. Rev.* 41, 6730–6744 (2012)
- 3. Pregelj, M., Zorko, A., Zaharko, O., Arčon, D., Komelj, M., Hillier, A. D., Berger, H.: Persistent spin dynamics Intrinsic to amplitude-modulated long-range magnetic order. *Phys. Rev. Lett.* 109, 227202-1-5 (2012)
- 4. Novak, N., Pirc, R., Wencka, M., Kunnjak, Z.: High-resolution calorimetric study of Pb Mg _{1/3} Nb _{2/3} O₃ single crystal. *Phys. Rev. Lett.* 109, 037601-1-5 (2012)
- 5. Zupančič, B., Diez-Berart, S., Finotello, D., Lavrentovich, O. D., Zalar, B.: Photoisomerization-controlled phase segregation in a submicron confined azonematic liquid crystal. *Phys. Rev. Lett.* 108, 257801-1-5 (2012)
- Vilfan, A.: Optimal shapes of surface slip driven self-propelled microswimmers. *Phys. Rev. Lett.* 109, 128105-1-5 (2012)
- Hwang, W. S., Remškar, M.: Transistors with chemically synthesized layered semiconductor WS₂ exhibiting 10⁵ room temperature modulation and ambipolar behavior. *Appl. Phys. Lett.* 101, 013107-1-4 (2012)
- 8. Essone Mezeme, M., Kranjc, M., Bajd, F., Serša, I., Brosseau, C., Miklavčič, D.: Assessing how electroporation affects the effective conductivity tensor of biological tissues. *Appl. Phys. Lett.* 101, 1–4 (2012)
- 9. Bajd, F., Vidmar, J., Fabjan, A., Blinc, A., Kralj, E., Bizjak, N., Serša, I.: Impact of altered venous hemodynamic conditions on the formation of platelet layers in thromboemboli. *Thromb. Res.* 129, 158–163 (2012)

Awards and appointments

- 1. Matjaž Gomilšek: Prešeren Award of the Faculty of Mathematics and Physics for Diploma thesis, University of Ljubljana, Ljubljana, Time irreversible billiards
- 2. Primož Koželj: Best paper award, Ljubljana, The European Integrated Center for the Development of New Metallic Alloys and Compounds, C-MAC days 2013, Ljubljana
- 3. Zdravko Kutnjak: Mentor awards in 2013, the Society of Young Researchers Slovenia

Organization of conferences, congresses and meetings

1. "C-MAC days 2013", Ljubljana, Slovenia, 9.-12. 12. 2013

Patent granted

- 1. Janez Pirš, Matej Bažec, Silvija Pirš, Bojan Marin, Bernarda Urankar, Dušan Ponikvar, Variable contrast, wide viewing angle LCD light-switching filter, US8542334 (B2), US Patent Office, 24.9.2013.
- S. G. Psakhie, Volia Isaevich Itin, D. A. Magajeva, O. G. Terehova, E. P. Najden, Olga Vasiljeva, Georgij Mihajlov Andrejevič, Urška Mikac, Boris Turk, Contrast agent for T1 and/or T2 magnetic resonant scanning and method for preparing it, RU2471502 (C1), Federal'naja služba po intellektual'n'noj so'stvennosti, 10.1.2013.
- 3. Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih, Procedure for synthesis of threadlike tungsten oxide W5014, US8496907 (B2), US Patent Office, 30.7.2013.

INTERNATIONAL PROJECTS

- MERCK AFM Investigations 1. Merck KGaA
 - Asst. Prof. Miha Škarabot
- 7FP DIAGNO-RAIL; Combining Innovative Portable Visual, Accoustic, Magnetic and 2. NMR Methods with In-situ Chemical Diagnostic Tools for Effective Failure Assessment and Maintenance Strategy of Rail and Subway Systems European Commission
- Prof. Janez Dolinšek 7FP LEMSUPER; Light Element Molecular Superconductivity: An Interdisciplinary 3. Approach
 - European Commission Prof. Denis Arčon
- 4. 7FP - ESNSTM; Electron Spin Noise Scanning Tunneling Microscopy European Commission
- Prof. Janez Dolinšek
- 5. 7FP - NanoMag; Magnetic Nanoparticles and Thin Films for Spintronic Applications and High Performance Permanent Magnets
- European Commission Prof. Janez Dolinšek
- 6. 7FP - NEMCODE; Controlled Assembly and Stabilisation of Functionalised Colloids in Nematic Liquid Crystals
- European Commission Prof. Igor Muševič
- COST MP1003; ESNAM European Scientific Network for Artificial Muscles COST Office
- Prof. Boštjan Zalar
- COST; IMC-SRM; Network for Intermetallic Compounds as Catalysts for Steam Reforming of Methanol COST Office
- Prof. Janez Dolinšek
- NATO ARW 984375; Magnetic Resonance Detection of Explosives and Illicit Materials, 2.-7.9.12, Turkey
- NATO North Atlantic Treaty Organisation Asst. Prof. Tomaž Apih
- 10. COST MP1201; Rational Design of Hybrid Organic-Inorganic Interfaces: The Next Step Towards Advanced Functional Materials COST Office
 - Dr. Polona Umek
- 11. Factor Xa Dimerization and Its Role in Prothrombinase Complex Formation and Activity on Membrane Surfaces Slovenian Research Agency
- Dr. Marieta Šentiurc
- 12. Syntesis, Microscopy Characterization and Magneto Resonance Study of New Functional Nanomaterials Slovenian Research Agency
 - Dr. Polona Umek
- 13. Unconventional Ground States of Quantum Matter Slovenian Research Agency Dr. Martin Klanjšek
- 14. Exotic Electronic Properties arising from Geometrical Symmetry Slovenian Research Agency Prof. Denis Arčon
- 15. Physiological Role of Factor Xa and Protein S in Coagulation and Inflammation Slovenian Research Agency
- Dr. Tilen Koklič 16. Novel Polymeric and Ionomeric Materials with Giant Dielectric and Electrocaloric Response
 - Slovenian Research Agency Asst. Prof. Vid Bobnar
- 17. Liquid Crystals Blue Phases in Confined Geometries: Structure, Optical Properties and Photonic Applications Slovenian Research Agency
- Prof. Igor Muševič
- 18. Elastically Tuned Soft Nanocomposites Slovenian Research Agency Prof. Samo Kralj
- 19. Promotion of Science and Cooperation of International Scientific Associations European Commission Prof. Igor Muševič

RESEARCH PROGRAMS

1. Magnetic Resonance and Dielectric Spectroscopy of "Smart" New Materials Prof. Janez Dolinšek

- Physics of Soft Matter, Surfaces and Nanostructures 2 Prof Slobodan Žumer
- 3. Experimental Biophysics of Complex Systems Prof. Igor Serša

R&D GRANTS AND CONTRACTS

- New Metallic Materials for Thermal Storage of Digital Information 1. Prof. Janez Dolinšek
- 2. Design, Formulation and Characterization of Biomimetic Nanocomposite Systems for Effective Tissue Regeneration Dr. Mojca Urška Mikac
- Theory of the Nematic Nanodroplet and Ordering of DNA, Encapsidated in Simple 3. viruses
- Asst. Prof. Andrej Vilfan Collective and Molecular Dynamics of Photosensitive Liquid Crystal Elastomers 4. Prof. Boštjan Zalar
- 5. Use of Green Energy Sources: New Functional Nanomaterials on the Base of Polyoxometalates and TiO2 Nanostrucutres for Production of Hydrogen by Catalytic Oxidation of Water -NANOleaf Dr. Polona Umek
- 6. Oligomers of Amyloidogenic Proteins from A to Z: Biophysical Properties, Structure, Function and Mutual Interactions
- Asst. Prof. Miha Škarabot 7 Optimization Strategies in Biological and Artificial Microfluidic Systems Asst. Prof. Andrej Vilfan
- Selective and Hipersensitive Microcapacitive Sensor System for Targetted Molecular Detection in the Atmosphere
- Prof. Igor Muševič 9. Textured Ceramic Layers for Sensors and Actuators
- prof. dr. Zdravko Kutnjak 10.
- Optical Microresonators Based on Liquid Crystals Prof. Igor Muševič
- 11. Biotechnological Processes of Treatment of Lignocellulosic Materials Prof. Janez Štrancar
- 12. Behaviour of Disipative Systems Under Extreme Termo-Mechanical Loading Dr. Andrei Zorko
- Water Exclusion Efficacy, Measure for Prediction of Wood Performance against Wood 13. Decay Fungi Prof. Igor Serša
- 14. New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics Prof. Boštjan Zalar
- 15. A Spectrometer for Automatic 14N Nuclear Quadrupole Resonance Characterization of New Substances Dr. Alan Gregorovič
- 16. Exchange Interactions in Selenides and Tellurides Key for New Functional Low-Dimensional Magnetic Systems Dr. Matej Pregelj
- 17. TABANA: Targeting AntimicroBial Activity via micro/Nano-structured sufaces for civil Applications
- Prof. Janez Štrancar 18. Nanomaterials and Scaffolds Preparation and Sharacterization Prof. Ianez Štrancar
- 19. New Polymer and Ceramic Materials for Potential Use in Capacitors Dr. Andreja Eršte
- 20. Influence of Mechanical Field on Electrical Properties of Oxide Semiconductor Materials Dr. Nikola Novak
- 21. Irradiation and Analysis of Si Samples Prof. Igor Muševič

NEW CONTRACTS

- 1. Protocol for Validation of the Analytical Method Lek d. d.
 - Asst, Prof. Miha Škarabot
- A Spectrometer for Automatic 14N Nuclear Quadrupole Resonance Characterization of 2. New Substances Gorenje Gospodinjski Aparati d.d.
- Dr. Alan Gregorovič
- Balder Technology Development 3. BALDER d.o.o.
- Prof. Igor Muševič
- Behaviour of Disipative Systems under Extreme Termo-Mechanical Loading 4 BALDER d.o.o. Prof. Igor Muševič

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- Dr. Adam Ostrovski, Poland, EUFP7 project "ESR-STM", 1. 11. 2012-31. 10. 2013 2
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- Silvio Preda, Ilie Murguescu Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania, 14.-25. 1. 2013
- Prof. Yishay Manassen, Ben Gurion University, Beer Sheva, Israel, 5.–12. 2., 17. 9. 2013 Prof. David Sherrington, University of Oxford, Oxford, Great Britain, 13.–14. 2. 2013 8.
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- 16. Prof. Igor Serša
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- 23. Dr. RamaRao Partibho, Raman Research Institute, Bangalore, India, 7. 9.-21. 9. 2013.
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- 25. Prof. Qiming Zhang, University of Pennsylvania State, Pennsylvania, USA, 18.-21. 9. 2013
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- 36. Dr. Jun-ichi Fukuda, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, 18. 12. 2013-11. 2. 2014

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66.

75.

77.

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Note:

Annual Report 2013

63. Dr. Adam Ostrowski, left 01.11.13

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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. These include anything from nano-biosystems to magnetic systems and superconductors. The experimental methods used are suitably diverse, from synthetic chemistry to femtosecond laser spectroscopy. Last year's research achievements are thus quite diverse, but we are able to report on breakthroughs in a number of areas.

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

In 2013 we spent a lot of effort on setting up new mid- and long-term research projects, which was started in the past two years. In particular, new techniques were developed for the study of non-equilibrium phase transitions, involving both theoretical and experimental work. This already paid dividends in the form of a number of break-through publications published in 2013, or to appear early in 2014. Most notable of the already published works is the publication in *Nature* on the discovery of a ferromagnetic liquid crystal composite by Alenka Mertelj et al., described in more detail below. Similarly, our pioneering forays into sample preparation yielded results with the publication of a paper by Jure Strle and co-workers in *Nature Materials* on molecular-beam-epitaxy-grown thin films. Notable publications in 2013 include the first observation of intrinsic and extrinsic topological defect dynamics in *Physical Review Letters* by T. Mertelj et al. Other notable publications on various subjects are listed below.

A significant amount of work was devoted to setting up new equipment made available by the Centre of Excellence in Nanoscience and Nanotechnology – Nanocenter. The department thus acquired a new AFM/Micro-Raman system with low-temperature vacuum capability, and a significant share and leading role in the running of a FIB dual-beam microscope, both of which are currently fully operational. In addition, in 2013 we continued the development of a new, low-temperature, four-probe STM/AFM system with Omicron, which is a unique instrument enabling unprecedented 4-contact measurements of surface transport on the nanoscale. A prototype version was installed in November of 2013 and a final version will be delivered early in 2014. An atomic layer deposition system was set up and tested, and is giving excellent results with the successful demonstration of a MoS2 nanotube fieldeffect transistor with comparable performance to the revolutionary MoS2 single-layer transistors reported by Kis et al. in 2010 from EPFL.

Ultrafast studies of electron dynamics in correlated systems

The field of research of relaxation processes of photo-excited electrons in correlated electron systems is one of our most advanced research topics. One part of this research includes the development of new methods, instrumentation and ultrafast laser systems for spectroscopy. New femtosecond techniques are thus being developed, such as multipulse spectroscopy and broad-band optical probe spectroscopy.

The research encompasses many different areas of physics and materials science. The most advanced part of the research takes place in conjunction with an ERC Advanced Grant on "Coherent trajectories through symmetry breaking transitions" which started in the first part of 2103. This work is challenging both conceptually and practically, and is still at an embryonic stage. Much of this work is thus still in the exploratory stage and not considered for publication as yet. The general framework is within the scope of "Cosmology in the lab experiments", coming from the analogy with the Big bang in cosmology or collisions in elementary particle physics in which phase transitions also take place in time from a highly excited plasma, much in the same way as phase transitions take place after the excitation of collectively

Several experimental studies of carrier relaxation phenomena in correlated electron systems with various degrees of correlation have been performed using femtosecond time-resolved techniques. The aim of the ongoing research is to gain additional information about the nature of the low-lying excitations in these materials, and to explore the nature and strength of the interactions of electrons with other low-lying excitations.



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ordered states in electronic systems which we investigate here. One of the novelties in these investigations relates to the study of non-equilibrium transitions in which the single particle and collective excitations are not in thermal equilibrium with each other and cannot be described in terms of a common temperature. Under such non-ergodic conditions the system trajectory is expected to be different than under ergodic conditions, and represent an absolute novelty, opening the way to unexplored new physics.

At the other end of the spectrum, femtosecond laser spectroscopy has developed over the years from an exotic experimental technique to a mainstream characterisation tool in materials science. The technique is now used to characterise the band structure of different materials, offering some unique insights that are not available with other spectroscopy techniques. For example, different excitations can be distinguished by their different lifetimes, thus allowing pseudogap excitations to be distinguished from a spin or superconducting gap.

Several experimental studies of carrier relaxation phenomena in correlated electron systems with various degrees of correlation have been performed using femtosecond time-resolved techniques. The aim of the ongoing research is to gain additional information about the nature of the low-lying excitations in these materials, and to explore the nature and strength of the interactions of electrons with other low-lying excitations.

We continued our research of the relaxation of quasiparticles in iron-based pnictide superconductors. We systematically investigate the photo-excited (PE) quasi-particle (QP) relaxation and low-energy electronic structure in an electron-doped, 1111-structure $Sm(Fe_{0.95}Co_{0.07})AsO$ single crystal. We found that the behaviour is qualitatively identical to the 122-structure $Ba(Fe,Co)_2As_2$ including the presence of a normal state pseudogap and a marked twofold symmetry breaking in the tetragonal phase that we relate to the electronic nematicity. The twofold symmetry breaking appears to be a general feature of the electron-doped iron pnictides. The results were published in Phys. Rev. B 87, 174525 (2013).



Figure 1: FET transistor, based on MoS2 nanotubes.

We continued the analysis of previously measured temperature and magnetic-field-dependent photo-excited electron and spin relaxation in $EuFe_2(As_{0.7}P_{0.3})_2$ (EFAP) pnictide superconductor and parent non-superconducting $EuFe_2As_2$ (EFA) by means of near-infrared optical pump-probe femtosecond spectroscopy. In both samples we observe at low temperature the emergence of a slow anisotropic photo-induced relaxation component concurrent with Eu2+ spin ordering. The slow dynamics of this component suggests a weak coupling between the Eu2+ spins and the carriers in the Fe-d derived bands.

The magnetic field dependence of the relaxation in the superconducting EFAP is different than in the non-superconducting EFA. In EFA we observe switching of the optical-transients anisotropy with an increasing magnetic field attributed to a field-induced antiferromagnetic-to-ferromagnetic phase transition. In the superconducting EFAP a large coherent magnon oscillation is observed at a similar metamagnetic transition. A short paper on some of the above results is in print in Optics and Spectroscopy, while a manuscript describing the majority of the results is in preparation.

A remarkable change of the quasiparticle relaxation dynamics at the antiferromagnetic SDW transition temperature in EFA and related $BaFe_2As_2$ and $SrFe_2As_2$, observed previously by the near-infrared probe, was systematically investigated by broad-band visible time-resolved spectroscopy. Two different relaxation processes were identified. The behaviour of the slower process, which is strongly sensitive to the magneto-structural transition, is consistent with the relaxation-bottleneck model involving magnons. Manuscripts describing the results are in the final stage of preparation.

In collaboration with Hokkaido University, Sapporo, Japan we investigated the dynamics of excitations with different symmetry in the superconducting (SC) and normal state of the high-temperature superconductor $Bi_2Sr_2CaCu_2O_{8*d}(Bi2212)$ using optical pump-probe (Pp) experiments with different light polarizations at different

The observation of distinct selection rules for SC excitations, present in A1g and B1g symmetries, and for the pseudogap excitations, present in A1g and B2g symmetries, by the probe and absence of any dependence on the pump beam polarization leads to the unequivocal conclusion of the existence of a spontaneous spatial symmetry breaking in the pseudogap state. doping levels. The observation of distinct selection rules for SC excitations, present in A1g and B1g symmetries, and for the pseudogap excitations, present in A1g and B2g symmetries, by the probe and absence of any dependence on the pump beam polarization leads to the unequivocal conclusion of the existence of a spontaneous spatial symmetry breaking in the pseudogap state. A manuscript describing the work was submitted to Phys. Rev. Lett. and is in the reviewing process.

A significant effort was invested into an investigation of the dynamical phase transitions in superconducting and CDW systems. The control of condensed-matter systems out of equilibrium by laser pulses allows us to

investigate the system trajectories through symmetry-breaking phase transitions. Thus the evolution of both collective modes and single-particle excitations can be followed through diverse phase transitions with femtosecond resolution. We presented experimental observations of the order parameter trajectory in the normal \rightarrow superconductor transition and charge-density wave-ordering transitions. Of particular interest is the coherent evolution of topological defects forming during the transition via the Kibble-Zurek mechanism, which appears to be measurable in optical pump-probe experiments. Experiments on CDW systems reveal some new phenomena, such as coherent oscillations of the order parameter, the the creation and emission of dispersive amplitude modes upon the annihilation of topological defects, and mixing with weakly coupled finite frequency (massive) bosons as described in J. Phys.: Condens. Matter 25, 404206 (2013). The paper was written at the invitation of Tom Kibble, and the entire journal issue was devoted to Cosmology in the laboratory experiments in his honour. The paper also reveals some new ideas concerning dark-matter excitations within the phase-transition picture and discusses the observation of the annihilation of domain walls and the ensuing emission of Higgs bosons detected in *lithography technique*. femtosecond optical experiments.



We extended previous investigations of Bi₂Sr₂CaCu₂O₈₊₄ cuprate superconductors by means of the 3-pulse timeresolved optical spectroscopy technique to different doping levels. The characteristic footprint of the superconducting response was also detected at temperatures above Tc, indicating the presence of the superconducting fluctuations up to 23 K above Tc, and are distinct from the excitations in the pseudogap state, which are observable up to T =200~250 K. We empirically establish the direct correspondence between the bare superfluid density as measured by the THz spectroscopy and the optical pump-probe response near Tc. The lifetime of both, the order parameter recovery associated with the superconducting fluctuations and quasiparticle recombination, is observed to diverge as T goes to Tc. The critical behaviour of the lifetime significantly differs from the time-dependent Ginzburg-Landau theory prediction for Gaussian fluctuations and phase correlation time measured by a.c. conductivity. The manuscript with the results is in the final stage of preparation.

In CDW systems we studied the incoherent recombination of topological defects created during a rapid quench of a charge-density-wave system through the electronic ordering transition. Using the above mentioned 3-pulse femtosecond optical spectroscopy technique we follow the evolution of the order parameter over a wide range of timescales after the quench. By careful consideration of thermal processes we clearly identified the intrinsic topological defect annihilation processes in TbTe, on a timescale of \sim 30 ps and found the signature of extrinsic defect-dominated relaxation dynamics occurring on longer timescales. A similar effect was also observed in blue bronze and 2H-TaSe₂. The results were published in Phys. Rev. Lett. 110, 156401 (2013).

The achievement of optical bistable switching between collective states of matter by non-thermal processes has great potential applications, but has so far been very elusive. Commonly, the photo-excited states are transient, and do not show true switching behaviour. After we have shown for the first time complete switching in 1T-TaS2 between the ground state and a new stable hidden state by a single laser pulse, we continued the investigation of the stability and transport properties of the switched state in thin 1T-TaS2 flakes adhered to various substrates by Van der Waals forces. A manuscript describing the major results is currently in the review process at Science

A prerequisite to perform femtosecond electron diffraction on modern quantum materials such as 1T-TaS2 is the availability of laterally large ($\sim 100 \,\mu$ m) and sufficiently thin ($< 100 \,$ nm) single-crystalline samples. Different approaches to reach these specifications have been tried out and their effect on sample integrity has been investigated. Finally, using an ultra-microtome, we were able to prepare 30 nm free-standing single-crystalline films of 1T-TaS2 with lateral dimensions of 200 µm × 200 µm. We have characterized these films with different techniques for their stoichiometric and crystalline integrity, ensuring no measurable alternation of the sample properties. The application of this sample-thinning technique is expected to find its use in further structural dynamics studies, as well as in optical time-resolved studies where homogeneous excitation profile and/or data in transmission geometry may be required. as reported in Ultramicroscopy 127, 9 (2013)

A table-top, femtosecond, non-relativistic, electron-diffraction setup is combined with a low-jitter, photo-triggered streak camera to follow the optically induced structural dynamics in complex solids. A temporal resolution of 550 fs is experimentally demonstrated, while the route to streaking with sub-250 fs temporal resolution is outlined. The technique is demonstrated by studying a photo-induced charge-density wave phase transition in 4Hb-TaSe2. Within the same data-acquisition time a three-fold increase in the signal-to-noise ratio is achieved when compared to the scanning method, with ways for a further improvement outlined. Appl. Phys. Lett. 102, 121106 (2013)

Theoretical studies on the nanoscale

We study theoretically how the dynamics of the resistive state in narrow superconducting channels shunted by an external resistor depends on the channel's length, the applied current, and parameter u characterizing the penetration depth of the electric field in non-equilibrium superconductors. We show that changing u dramatically affects both the behavior of the current-voltage characteristics of the superconducting channels and the dynamics



Figure 3: Micrometer contacts on a sample of TaS_x made with the laser lithography technique.



Figure 4: MoN nanowire with four Pt measuring contacts, which are prepared using FIB-assisted deposition.



Figure 5: FIB fabricated TEM lamella. Thickness is in the range of 60–80nm.

of their order parameter. Depending on the value of the parameter u the current-voltage characteristic may be step like or hysteretic. Shunting the superconductor with the resistor leads to the disappearance of the hysteretic current-voltage characteristic. (Physical Review B 87, 174516 (2013)).

We present a detailed analysis of the time-resolved optical data on blue bronzes (K_{0.3}MoO₃ and Rb_{0.3}MoO₃), prototype quasi-one-dimensional chargedensity wave systems. Numerous coherent (Raman active) modes appear upon the phase transition into the CDW state. We analyze the temperature dependence of the mode frequencies, their damping times, as well as their oscillator strengths and phases using the time-dependent Ginzburg-Landau model. We demonstrate that these low-temperature modes are a result of the linear coupling between the Fermi surface nesting driven modulation of the conduction electron density and the normal-state phonons at the CDW wave vector, and determine their coupling strengths. We were able to identify the nature of the excitation of these coupled modes, as well as the nature of the probing mechanisms in this type of experiments. We demonstrate that in incommensurate CDW systems, femtosecond optical excitation initially suppresses the electronic density modulation, while the reflectivity changes at frequencies far above the CDW-induced gap in the single-particle excitation spectrum are governed by the modulation of interband transitions caused by lattice motion. (Physical Review B 89, 045106 (2014)).

Nanomaterials

Nanowires and nanotubes decorated with gold nanoparticles are known for their excellent sensing and catalytic properties. However, the decoration of transition-metal dichalcogenide nanotubes can be very complex. We have found a simple procedure that enables the efficient production and purification of thin bundles of MoSi nanowires decorated with gold nanoparticles and their transformation to gold-decorated MoS, nanotubes. We isolated several hundred milligrams of nanowire bundles that were several microns long with average diameters of around 40 nm, and formed a stable dispersion in water without added surfactants. Gold nanoparticles were directly deposited on the nanowire bundles, either in a solution or on a substrate at room temperature in a single-step reaction without any additional reducing reagents The described procedure is one of the few examples of redox templating at room temperature without the use of a reducing agent to produce metal-decorated nanowires. The number of gold nanoparticles on a nanowire bundle is controlled by changing the concentration of chloroauric acid HAuCl₄ in the solution. Since the nanowires can serve as precursor crystals for the fabrication of nanotubes, we were able to transform gold-decorated nanowires and produce gold-decorated MoS, nanotubes. These results are reported in J Nanopart Res (2013) 15:1791

Electron dynamics in biological macromolecules

In 2013 we concluded our experimental work on dc electron transport in DNA and its complex with transition-metal cations – M-DNA. Transport measurements were performed on micron-sized electric circuits produced by e-beam lithography with parallel gold electrodes. The electrodes were separated by a several hundred nanometers wide gap (typically 250–500 nm). The gap was bridged with individual DNA molecules that were cast from a buffer solution onto the silicone chip surface.. Such single molecule electric nanocircuits have enabled us to measure the I-V characteristics of individual DNA/M-DNA molecules under ambient conditions as well as the temperature dependences of their electrical conductivity in a broad temperature range (20–300 K). The measurements have shown that the conductivity of a pristine DNA exhibits an activated behavior where the conductivity exponentially decays towards zero as the temperature is lowered from room temperature – a behavior typical for electric insulators. In contrast, the conductivity of an M-DNA molecule has shown a plateau in the middle temperature range (100–200 K) where the conductivity is virtually temperature-independent. These results give a firm support to a hypothesis that the electron transport in M-DNA is strongly correlated and much more efficient at longer (> 10 nm) distances then in the native DNA.

Thin-film synthesis and characterization

In 2013 we gained access to new thin-film synthesis techniques – Molecular Beam Epitaxy (MBE) and Atomic Layer Deposition (ALD).

One of the intensely studied scenarios of high-temperature superconductivity (HTS) postulates pairing by the exchange of magnetic excitations. In the heavily overdoped regime, neutron scattering measurements indicate that magnetic excitations have effectively disappeared, and this has been argued to cause the demise of HTS with overdoping. We have used resonant inelastic X-ray scattering to measure the evolution of magnetic excitations in $La_{2x}Sr_xCuO_4$ across the entire phase diagram, from a strongly correlated insulator to a non-superconducting metal ($0 \le x \le 0.40$). For x = 0, well-defined magnon excitations were observed. These magnons broaden with doping, but they persist with a similar dispersion and comparable intensity all the way to the non-superconducting, heavily overdoped metallic phase. We have concluded that the destruction of HTS by overdoping is caused neither by the general disappearance nor by the overall softening of magnetic excitations. These results were produced in collaboration with Brookhaven National Laboratory where we have performed sample characterization, and were reported in *Nature Materials 12, 1019-1023 (2013)*.

Soft Matter

Also in 2013 we continued with investigations of optical holographic patterning in light-sensitive liquid-crystal elastomers (LCEs). These are polymer materials that exhibit a very strong opto-mechanical response, due to which they are promising for applications in various optically manipulated micromechanical devices. We performed a comparative study of UV-irradiation-induced refractive-index modulation in two analogous monodomain nematic side-chain LCE materials. In one of them mesogenic azobenzene derivatives were incorporated as pendant co-monomers, and in the other as crosslinking units. The results are reported in the paper *Macromol. Chem. Phys.* 214, p. 2744 (2013). We also completed the investigation of optical-patterning properties in the vicinity of nematic-paranematic phase transition and reported our results in *Phys. Rev. E*, 87, p. 022507 (2013).

We completed our investigation of the effect of inorganic nanotubes and nanowires on the electro-optical properties of standard nematic liquid crystals. The results are reported in the paper *Phys. Status Solidi. A 210, p. 2328 (2013)*. We also studied the inclusion of MoS₂ nanotubes into polymerizable nematic liquid crystal material RM257 (Merck) and successfully fabricated a polymer-nanotube composite material with strongly aligned nanotubes.

In cooperation with TEDA APS at Nankai University (China) we investigated surface structure modifications of silicon induced by irradiation with a single femtosecond laser pulse and the possible application of the resulting surface structures for surface-enhanced Raman scattering. The results were reported in *J. Raman Spectrosc.* 44, p. 1678 (2013) and Optics Letters 39, p. 343 (2014). Another topic of our cooperation was the investigation of intracellular processes in biological cells. We investigated correlations of the fluctuations of calcium ion concentration between different cells and temperature-induced modifications of radiative activity of fluoropores sensitive to calcium ions. The results were published in *Biochem. Biophys. Res. Commun.* 431, p. 664 (2013) and *Biochem. Biophys. Res. Commun., in-press,* (2014).

In cooperation with the Center of Excellence for Polymer Materials and Technologies (PoliMaT) we performed a systematic analysis of the effect of oxygen plasma on the water-sorption properties of cellulose fibers. We demonstrated that modifications of optical birefringence of the fibers can be conveniently used to monitor the kinetics of the sorption process. The results were reported in *Carbohydrate Polymers 97, p. 143 (2013).*

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



Figure 6: The cover of the magazine Macromolecular Chemistry and Physics. Author of the picture: Irena Drevenšek Olenik

We completed a comparative study of the aggregation properties of four similar guanine (G)-rich DNA oligonucleotides.



Figure 7: The growth-mechanism of guanine-based nanowires (G-wires) is preferably G-quartet stacking while GC-base pairing proved to be highly limited.

We showed that in an ordered nematic liquidcrystalline phase of the suspension of BaHF nanoplatelets doped with Sc in liquid-crystal 5CB ferromagnetic ordering appears.



Figure 8: A schematic presentation of the distortion of the director (blue) and magnetic field (orange) around disk-like platelets (short, thick horizontal lines) represented side-on. Blue dots indicate cross-sections of disclination lines, and red arrows the directions of magnetic moments.

We completed a comparative study of the aggregation properties of four similar guanine (G)-rich DNA oligonucleotides in a collaboration with the National Institute of Chemistry, Ljubljana and the University of Ulster, UK. The results show that all the investigated oligonucleotides assemble into G-quadruplex structures. But, in contrast to the expected behaviour, oligonucleotides without the "sticky" GC ends form shorter G4-wire structures than the oligonucleotides without the GC ends. The results were reported in *J. Phys. Chem. C 117, p. 23208 (2013).* Our research work on G-quadruplex related molecular self-assembly was also published in two chapters in the monographic publication: "*Guanine quartets: structure and application*", *edited by W. Fritzsche and L. Spindler (RSC Publishing, Cambridge, UK, 2013).*

We showed that in the ordered nematic liquid-crystalline phase of the suspension of BaHF nanoplatelets doped with Sc in liquid-crystal 5CB ferromagnetic ordering appears. The magnetization is along the nematic director and comes from the ferromagnetic ordering of the nanoplatelets. When the sample is prepared in the absence of an external magnetic field, two types of magnetic domains appear with magnetizations in the opposite directions. If during the preparation an external magnetic field along the director is applied, a monodomain sample is obtained. Magnetization curves show that a small magnetic field is needed to switch the domains. In samples with a low concentration of magnetic platelets the memory of the initial magnetic state of the sample is preserved and after the removal of the external field, the sample relaxes back to its initial magnetic state, while in samples with a high enough concentration a complete reversal of magnetization can be observed. During this complete reversal the travelling of the domain walls at the sample surface can be observed. The results are reported in Nature 504, 237-241 (2013).

Nonlinear optics

In the Nonlinear Optics Laboratory we study new materials and their interaction with laser light. Integrated optics is a promising technology; however, better materials will increase its potential. In cooperation with North Carolina State University in Raleigh, USA, we study new concepts of compact light sources on the basis of the nonlinear optical conversion of existing lasers into the spectral regions where lasers are not yet available. AlGaN grown by metal-organic chemical vapor deposition (MOCVD) has a great potential for optoelectronic devices emitting and detecting light in the ultraviolet (UV) wavelength regime. We study AlGaN waveguides with an alternating sign of the nonlinear coefficient in regular intervals and allows quasi phase matching.

The terahertz spectrum offers a broad range of applications in the chemical sensing and non-destructive testing of materials impenetrable by infrared or visible light. Broadband THz pulses may be generated by using femtosecond laser pulses combined with photoconductive switches and semiconductor surfaces, as well as by optical rectification in nonlinear optical crystals. The total THz power generated with these techniques is distributed over a broader spectral range. To obtain reasonable power at a certain THz frequency, a narrower band pulsed output with a high beam peak power is preferred. In cooperation with Rainbow Photonics A.G., a spin-off company of ETH Zurich, we study THz generation with difference frequency mixing. We developed a compact two-frequency laser where the two frequencies are generated in Nd:YAG and Yb:YAG branches of a split laser resonator with a common Q-switch and an output coupler. The emission wavelengths at 1.03 μ m and 1.06 μ m are mixed in a stack of thin platelets of organic crystal OH1 using quasi-phase matching. The generated THz frequency of 9.3 THz

is sufficiently far away from the water absorption lines and therefore large propagation distances of the THz waves can be realized in devices, e.g., for remote materials testing.

Biomedical optics

We have investigated the potential of non-contact measurements of laser-induced temperature profiles in biological tissues based on pulsed photo-thermal radiometry (PPTR). Using a laboratory PPTR setup, we have monitored the laser removal of tattoos in human volunteers. We have demonstrated the relevance of the obtained information for studies of the interaction process and guidance of therapy on an individual patient basis.

Using the same technique, we have characterized the interaction of a prototype Nd:YAP laser (1342 nm) with the skin of healthy volunteers, and compared it with two common medical lasers (Nd:YAG and KTP, emitting at 1064 and 532 nm, respectively). The results indicate that the Nd:YAP laser is very suitable for non-ablative rejuvenation of sun-damaged skin. Both studies were performed in collaboration with Fotona d.d., Ljubljana.

By combining the above experimental approach and a dedicated numerical model, we have developed an original method for the individual determination of the maximum safe radiant exposure in the irradiation of human skin with millisecond laser pulses. Our approach has great potential for improving the efficacy and safety of several dermatologic laser treatments. We have analyzed the influence of the acquisition sampling rate and noise characteristics of the infrared radiation detector on the procedure.

A similar approach was also adopted for a quantitative assessment of hemoglobin mass diffusion, physiological degradation rate, and depth of blood spill in traumatic bruises (hematomas). The obtained knowledge should enable the development of more accurate and reliable techniques for a determination of the time of injury in forensic science.

We have developed a three-dimensional (3D) Monte Carlo (MC) model of light transport in strongly scattering and heterogeneous human skin with a rigorous treatment of analytically defined boundaries between neighbouring tissues. In contrast with the common implementation of the 3D MC approach, where tissue boundaries are approximated according to the rectangular spatial grid, the results of our model do not depend on the positioning or discretization step of the spatial grid.

Non-invasive measurements of temperature profiles induced in healthy human skin with a prototype Nd:YAP laser have demonstrated the suitability of its 1342-nm emission for nonablative skin rejuvenation. (collaboration with Fotona d.d., Ljubljana)

We have studied the potential of diffuse reflectance spectroscopy (DRS)

for the non-contact characterization of biological tissues. We have developed an original approach for the rigorous elimination of a known artefact in measurements of DRS using an integrating sphere. We have analyzed the accuracy and robustness of DRS analysis using analytical solutions for the transport of light in strongly scattering tissues, derived within the so-called diffusion approximation. (Collaboration with NTNU, Trondheim, Norway).

Biological systems

We studied biomimetic systems, especially artificial cilia and artificial swimmers at low Reynolds numbers. The unique magneto-optical tweezers, which were used in the experiment, were developed at the Laboratory for Experimental Soft Matter, Faculty of Mathematics and Physics, University of Ljubljana. The fabrication of artificial cilia, the characterisation of generated fluid flows, the coupling between cilia and the fabrication of colloidal scaffold for cell growth were also the topics included in the thesis by young researcher Gasper Kokot, who successfully defended

his thesis "Measuring forces with magneto-optical tweezers in biological and biomimetic systems". Our work on artificial cilia also appeared in the book *Artificial Cilia*, published by the Royal Society of Chemistry, Cambridge, UK.

Biomimetic research also included systems of artificial swimmers. We studied different mechanisms that led to processive motion. The symmetry in the system was broken with the vicinity of the surface and different hydrodynamic drag on the individual components of the swimmer. We created isotropic swimmers that move in an arbitrary direction, not determined by the driving external magnetic field. Microswimmers achieved a velocity of several micrometers per second under optimal conditions. The experimental part of the research is completed, and in collaboration with the Department for Condensed Matter Physics (F5), numerical simulations are being done to explain the observed phenomena. Experimental work was presented at the International Soft Matter Conference in Rome and a paper is in preparation.

In collaboration with the Department for Condensed Matter Physics (F5) we also numerically investigated the energy efficiency of different beating patterns of artificial cilia. We have shown the importance of metachronal coordination for the generation of fluid flow above a densely ciliated surface



Figure 9: Periodically inverted domains of Al-polar and N-polar AlN forming an optical waveguide. Such a structure is used for nonlinear frequency conversion by quasi phase matching into the deep UV region.

and that even time-symmetric reciprocal motion enables pumping. The results were presented at two international conferences: Biophysical Society Meeting, Philadelphia, USA and at Dynein 2013 in Kobe, Japan.

We also continued our work on thermophoresis, which is carried out in collaboration with the group of Professor Braun, University of Munich, Germany. Thermal gradients were used to successfully move molecules of DNA and we have shown that the replication and accumulation of DNA can be implemented in the same micrometer-sized setting. This opens up a new approach to understanding the dynamic development of a molecular Darwinian system. The results of the investigations were published in the paper "Could Thermal Gradient Drive Molecular Evolution?", *Curr. Org. Chem. 17 1732 (2013).*

Some outstanding publications in the past year

- 1. Mertelj, A., Lisjak, D., Drofenik, M., Čopič, M.: Ferromagnetism in suspensions of magnetic platelets in liquid crystal. *Nature*, 2013, vol. 504, no. 7479, 237-241
- Mertelj, T., Kušar, P., Kabanov, V. V., Giraldo-Gallo, P., Fisher, I. R., Mihailović, D.: Incoherent topological defect recombination dynamics in tbte₃: T. Mertelj ... [et al.]. *Physical review letters* [print ed.], 2013, vol. 110, no. 15,156401-1-156401-5
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- 1. Čoga, L., Ilc, T., Devetak, M., Masiero, S., Gramigna, L., Spada, G. P., Drevenšek Olenik, I.: Liponucleoside thin films: the special behaviour of guanosine. *Colloids surf.*, *B Biointerfaces*. [print Ed.], 2012, vol. 103, 45–51
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Organization of conferences, congresses and meetings

1. SLONANO 2013, Ljubljana, Slovenia, 23.-25. 10. 2013, coorganizers

Patent granted

1. Andrej Kovič, Adolf Jesih, Aleš Mrzel, The procedure for the synthesis of 4d and 5d (Nb, Mo Ta, W) nitrites of transition metals in the form of quasi-one-dimensional structures, SI23988 (A), Urad RS za intelektualno lastnino, 30.8.2013.

INTERNATIONAL PROJECTS

- 1. Organization of the International Conference SLONANO 2013, Ljubljana, Slovenia, 23.-25. 10. 2013
 - Foreign Clients Prof. Dragan Dragoljub Mihailović
- 7FP HINTS; Next Generation Hybrid Interfaces for Spintronic Applications European Commission
- Prof. Viktor Kabanov
 7FP COSIT; Compact High Brilliance Single Frenquency Terahertz Source European Commission
- Prof. Marko Zgonik 4 7FP - MoWSeS Nanoelectronics based on Two-Dimensional
- 7FP MoWSeS; Nanoelectronics based on Two-Dimensional Dichalcogenides European Commission Asst. Prof. Christoph Gadermaier
- 7FP TRAJECTORY, Coherent Trajectories through Symmetry Breaking Transitions European Commission
- Prof. Dragan Dragoljub Mihailović
- 6. COINAPO; Composites of Inorganic Nanotubes and Polymers COST Office
- Prof. Dragan Dragoljub Mihailović
- 5th International Conference on Photoinduced Phase Transitions and Cooperative Phenomena - PIPT5, Bled, Slovenia, 9.-13. 6. 2014 Foreign Clients
- Prof. Dragan Dragoljub Mihailović
- Electron -phonon Coupling in High-Temperature Superconductors Determined from Femtosecond Electron Relaxation Rates Slovenian Research Agency Prof Viktor Kabanov
- Photonic Structures Based on Polymer-Nanoparticle Composites Slovenian Research Agency Prof. Irena Drevenšek Olenik
- 10. Crystal and Film Growth and Time-domain Optical Spectroscopy Investigations of the Supeconducting State of the Cuprate Superconductors

- 11. Slovenian Research Agency Asst. Prof. Tomaž Mertelj
- 12. Time Resolved Optical Spectroscopy of Collective Electronically Ordered States in Iron Based Phictides
 - Slovenian Research Agency Prof. Viktor Kabanov
- Spectrum of the Collective Excitations of the Quasi-one-dimensional Conductors with the Charge Density Wave in the Equilibrium and Nonequilibrium State Slovenian Research Agency Prof. Viktor Kabanov

RESEARCH PROGRAMS

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

R&D GRANTS AND CONTRACTS

- 1. Collective and Molecular Dynamics of Photosensitive Liquid Crystal Elastomers Dr. Matija Milanič
- 2. Cosmology in the Lab: Femtosecond Control of Phase Transitions in Real Time Prof. Dragan Dragoljub Mihailović
- 3. Optimization Strategies in Biological and Artificial Microfluidic Systems Asst. Prof. Andrej Vilfan
- Symmetry Breaking in Real Time Prof. Dragan Dragoljub Mihailović
- Center of Competence BioMedical Engineering: CC BME
- Prof. Boris Majaron 6. Development of New Ultrafast Change Memory Devices by Femtosecond Multi-pulse

Spectroscopy (ULTRA-MEM-DEVICE) Dr. Ljupka Stojčevska Malbašić

- COST MP1205; Advances in Optofluidics: Integration of Optical Control and Photonics 7. with Microfluidics
- Dr. Natan Osterman
- COST MP1302; NanoSpectroscopy 8 Asst. Prof. Christoph Gadermaier
- 9 Irradiation and Analysis of Si Samples Miloš Borovšak, B. Sc.

NEW CONTRACTS

- 1 Slovenian Tournament of Young Physicists Ames, d. o. o.
- Prof. Irena Drevenšek Olenik
- 5th International Conference on Photoinduced Phase Transitions and Cooperative 2 Phenomena - PIPT5, Bled, Slovenia, 9.-13. 6. 2014 Lek d d
- Prof. Dragan Dragoljub Mihailović
- 3. Organization of the International Conference SLONANO 2013 Lek. d. d.

Prof. Dragan Dragoljub Mihailović

- VISITORS FROM ABROAD
- Andrei Shumilin, Ioffe Physical-Technical Institute of the Russian Academy of Sciences, St. Petersburg, Russia, 11. 1.-10. 4. 2013
- Prof. David Sherrington, University of Oxford, Oxford, Great Britain, 13.-14. 2. 2013
- 3. Nataša Vujičič, Institute of Physic, Zagreb, Croatia, 4.-31. 3. 2013
- Dr. Sumeet Kumar, Innovation Factory SRL, Trieste, Italy, 5. 3.-31. 5. 2013
- Prof. Serge Brazovski, Prof. Nathalie Kirova Brazovski, Université Paris Sud, Paris, 5. France, 22. 4-20. 5. 2013
- Prof. Hans Kuzmany, University of Vienna, Vienna, Austria, 21.-22. 5. 2013 6.
- Prof. Xin Yao, Shanghai Jiao Tong University, Shanghai, China, 30. 5.-13. 6. 2013
- Prof. Zhuan Xu, Zhejiang University, Zhejiang Province, China, 15.-20. 6. 2013 8

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- 4 Prof. Viktor Kabanov
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- 14. Asst. Prof. Lea Spindler*
- 15. Dr. Mojca Vilfan
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- 22. Dr. Jure Strle
- 23. Dr. Martin Strojnik

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ORIGINAL ARTICLE

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- Katarina Tlučková, Faculty of Science, P. J. Šafarik University, Kosice, Slovakia, 11. 7. 2013 10. Cui Wei, Nakai University, Tianjin, China, 15. 7.-15. 8. 2013
- 11. Prof. Aleksander Balanov, Loughborough University, Loughborough, Great Britain, 30. 7.-1. 8. 2013
- 12. Daniele Vella, University of Pisa, Pisa, Italy, 28.-30. 8. 2013
- 13. Victor Vega, University of Salamanca, Salamanca, Spain, 26.-28. 8. 2013
- Prof. Jan Lagerwall, Prof. Guisy Scalia, Seoul National University, Seoul, South Korea, 16.-18.9.2013
- Andrei Shumilin, Ioffe Physical-Technical Institute of the Russian Academy of Sciences, 15 St. Petersburg, Russia, 15. 10.-15. 12. 2013

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Postgraduates

- 24. Miloš Borovšak, B. Sc.
- 25. Tetiana Borzda, B. Sc.
- 26. Jože Buh, B. Sc. Dr. Gašper Kokot, left 01.04.13
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- 29. Anna Pogrebna, B. Sc.
- 30. Matej Prijatelj, B. Sc.
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- 36. Petra Šutar, B. Sc.
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- 37. Martina Knavs, B. Sc.
- 38. Janja Milivojević
- 39. Nataša Zakrajšek, B. Sc.

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- 1. Lucija Čoga, Miha Devetak, Stefano Masiero, Gian Piero Spada, Irena Drevenšek Olenik, "Specific behaviour of guanosine in liponucleoside thin films", In: *Guanine quartets: structure and application*, Wolfgang Fritzsche, ed., Lea Spindler, ed., Cambridge, RSC Publishing, cop. 2013, pp. 154-163.
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PATENT APPLICATION

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PATENT

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MENTORING

- 1. Vladimir V. Baranov, *Dynamics of the resistive state in the nonequilibrium superconductors and relaxation of the hot electrons in metals:* doctoral dissertation, Ljubljana, 2013 (mentor Viktor Kabanov).
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- Ljupka Stojchevska, Femtosecond relaxation dynamics in collectiveelectronic-state materials: cuprate and iron-pnictide superconductors and charge-density wave systems: doctoral dissertation, Ljubljana, 2013 (mentor Tomaž Mertelj; co-mentor Dragan D. Mihailović).
- 4. Martin Strojnik, *Charge transport in MosS3Is nanowires and related systems:* doctoral dissertation, Ljubljana, 2013 (mentor Dragan D. Mihailović).
- 5. Tadeja Forjanič, *Reconstruction of tomographic images based on pulsed photothermal radiometry:* master's thesis, Ljubljana, 2013 (mentor Boris Majaron).
- 6. Peter Naglič, *Determination of human skin structure using diffuse reflectance spectroscopy:* master's thesis, Ljubljana, 2013 (mentor Boris Majaron).

DEPARTMENT OF REACTOR PHYSICS F-8

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

In the field of **reactor physics** we continued our research on the development of new methods for the analysis of research and power reactors.

In collaboration with CEA Cadarache a series of experiments was carried out at the TRIGA reactor for the determination of the kinetic parameters of the reactor. At the JSI TRIGA a simultaneous measurement with four fission cells was first performed and in parallel a new SPECTRON device, developed by the CEA, was also tested. Within the same project we improved the method of measuring the control rod worth using the rod-insertion method.

Within the scope of another project in collaboration with the CEA we tested the IRDFF neutron dosimetry Asst. Prof. Andrej Trkov library, to which we contributed previously. We compared the computational results with activation measurements on the TRIGA reactor in the process of neutron spectrum unfolding for different irradiation channels in the reactor.

In the framework of the environmental monitoring control for non-proliferation in nuclear Safeguards, the Department Analyse, Surveillance, Environment (DASE) of the Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA) has developed analytical techniques to detect traces of uranium and plutonium in micrometric particles. The method is called The Fission Track-Thermoionization Mass Spectrometry (FT-TIMS) and among others requires the irradiation of the sample under a well-thermalized neutron flux. The aim of the collaboration between CEA and the Jožef Stefan Institute in Slovenia is to develop an irradiation channel/device in the TRIGA reactor with the required neutronic characteristics, which will then be used for irradiation of CEA - DASE samples for the FT-TIMS method under well-defined conditions.

Our involvement in international projects included the evaluation of nuclear data and their covariance information. We completed the evaluation of the nuclear data file for ⁵⁵Mn and offered it to the OECD/NEA Data Bank for inclusion in the European JEFF-3.2 library, which will be released in 2015. We completed the selection of integral benchmarks for the validation of nuclear data for ²³⁸U and the isotopes of Fe and performed sensitivity/uncertainty calculations for selected test cases within the OECD/NEA Working Group WPEC SG-33.

The participation continued in the scope of the international projects of OECD/NEA UAM, WPEC-SG33, WPEC SG38, WPEC SG39 as well as the EC projects ANDES in F4E. The methodologies for nuclear data sensitivity and uncertainty analysis were further improved and applied to fission reactors (criticality safety studies, delayed neutrons, uncertainty in the effective delayed neutron fraction, in prompt and delayed fission neutron fraction) and the future fusion reactor ITER. In the area of benchmark experiments we started the cooperation on the new copper benchmark to be performed at the FNG DT facility in ENEA Frascati and continued the participation in the international shielding benchmark database SINBAD under development at OECD/NEA, covering the neutron/ gamma shielding experiment for fission, fusion and accelerator applications. In cooperation with the OECD/NEA and F4E we developed a computer environment facilitating the use of transport, sensitivity and uncertainty codes and the graphical package for the visualisation of sensitivity analysis results. In the scope of the UAM project of the OECD/NEA we organised an intercomparison study for the sensitivity codes based on the SNEAK critical experiments and proposed a similar intercomparison for the effective delayed neutron fraction.

Reactor Physics Department researchers also provided technical support in 2013 for the safe operation of the Krško nuclear power plant (NPP). We have independently confirmed nuclear design calculations for the fuel cycle 27 and performed start-up tests after the fuel reloading. As an authorised expert organization in the field of radiation and nuclear safety we performed an independent expertise on a NPP Krško reload safety evaluation for the cycle 27 and provided an expert review of the analysis and testing report for capsule T from the NPP Krško reactor vessel irradiation surveillance program.

In the field of **plasma physics** we have strengthened our collaboration with the University of Sofia in the development of a modern plasma characterization method with a Langmuir probe in magnetized plasma. This approach has been successfully implemented in measurements on the Compass tokamak. This work is also important



for plasma diagnostics in larger fusion devices and it complements well our work on the ball-pen type of probe and emissive probe for use in tokamaks. We collaborate in these two areas with IPP Prague and the University of Innsbruck. We have helped the latter to design an emissive probe for use in tokamaks and provided theoretical support. Therefore, our more fundamental research was still focused on the development of computational models of plasma in front of an electron-emitting electrode, but we also worked on gas-filled diode breakdown. A lot of work



Figure 1: Example of a resonance parameter correlation matrix. In figure: correlations between γ widths of ⁵⁵Mn resolved resonances from ENDF/B-VII.1 library (N=1 corresponds to lowest energy).

was done using computer simulations; we have successfully carried out a comparison between kinetic plasma simulations of our experimental device (a linear magnetized plasma device) with Langmuir probe measurements. We have also conducted simulations of plasma in front of an electrode for small potential drops, i.e., close to the plasma potential using a specially adapted particle-in-cell code.

In the field of **neutron transport calculations for fusion reactors**, we continued and expanded our work for JET - Joint European Torus, the largest fusion reactor. Co-workers of the Reactor Physics Division have, in collaboration with the JET stuff, performed calculations of the neutron field inside the torus for various past torus configurations (1986-2013) and thereby determined the differences in the historical response of the detectors. In doing so, we discovered a significant error in most of the past calculations of the detector response, arising from the limited computing capabilities of the 20th century, which could be eliminated with the use of the most recent techniques. The JSI researchers are co-responsible for the maintenance of a model of JET, to be used for transport calculations by the Monte Carlo method.

The calibration of detectors with a neutron source was one of the most important projects in JET in 2013, in which co-workers of F8 were responsible for the supporting calculations for the evaluation of the uncertainty of the calibration and the calculation of the corrections due to circumstances that are different during operation, e.g., additional structures inside and outside the Tokamak, neutron spectra, shape of the neutron source, etc.

The long-term work on the JET gamma ray camera was concluded with calculations of the attenuation of neutrons in the neutron attenuator of the horizontal camera and of the contribution due to the scattered neutrons within the attenuator.

The analysis of the Grenoble-led slowing-down experiment has been performed. One of the noticeable achievements was to optimize the limit between the resolved and unresolved resonance regions for the ¹⁹⁷Au cross-section.

Our research in the field of medical physics was focused in the analysis of Positron Emission Tomography (PET) images, image-guided cancer therapy and modelling. One significant part of our research work was dedicated to the research of fluorothymidine (FLT) tissue uptake stabilization during the PET imaging. We experimentally and theoretically demonstrated that the stabilization time for PET images is inversely proportional to the FLT tissue uptake parameters (SUV, the kinetic influx parameters), which could help in determining the optimal time interval for static PET imaging. Another part of our research work was dedicated to the comparison of two radiopharmaceuticals (sodium fluoride (NaF) and fluorodeoxyglucose (FDG)) for the PET-based evaluation of bone metastases treatment response. The basic finding was that the late NaF and FDG responses are consistently correlated, while earlier responses may be different. The third part of our research work (connected with the successful completion of a master's thesis) covered a modelling of tumour response to treatment with the anti-angiogenic targeted drug Axitinib. With our model we reproduced the reduction of cell proliferation during the therapy and proliferative flare after the therapy discontinuation, which was also experimentally verified. Clinical data for those three projects were obtained from the University of Wisconsin. We also worked on the development of an algorithm for a non-invasive determination of the input function (time dependence of radiopharmaceutical activity in the blood plasma) for kinetic modelling. We developed a novel algorithm, based on factor analysis, which was tested on experimental data obtained from The National Institute of Mental Health, USA. We have reliably determined the input function from the PET images even when the diameter of the largest artery in the field of view was comparable to the resolution of the PET scanner.

Some outstanding publications in the past year

 Žerovnik, G., Capote, R., Trkov, A.: On random sampling of correlated resonance parameters with large uncertainties. Nuclear instruments and methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, ISSN 0168-9002. [Print ed.], 2013, vol. 723, 89–98

- Žerovnik, G., Trkov, A., Smith, Donald L., Capote, R.: Transformation of correlation coefficients between normal and lognormal distribution and implications for nuclear applications. Nuclear instruments and methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, ISSN 0168-9002. [Print ed.], 2013, vol. 727, 33–39
- $\label{eq:scalar} 3. \quad \mbox{Kodeli, Ivan A.: Sensitivity and Uncertainty in the Effective Delayed Neutron Fraction ($\beta eff)$, Nuclear Instruments and Methods in Physics Research A 715(2013)70–78 }$
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INTERNATIONAL PROJECTS

- 1. Reports on Thermal Neutron Induced SEU Susceptibility of PXIe and cRIO Fast Controller Components ITER Organization
 - Dr. Luka Snoj
- 2. 7FP EURATÓM ANDES; Accurate Nuclear Data for Nuclear Energy Sustainability European Commission
- Asst. Prof. Andrej Trkov 3. F4E-FPA-168-01; Nuclear Data Improvements and Development of Tools - Nuclear Data Evaluation
- European Commission Prof. Ivan Aleksander Kodeli
- Specific Grant Agreement; Cu Experiment and TBM Nuclear Instrumentation European Commission
- Prof. Ivan Aleksander Kodeli 5. 7FP - CHANDA; solving CHAllenges in Nuclear Data European Commission
- Prof. Ivan Aleksander Kodeli
- 7FP EURATOM; Public Information; Research Unit Administration and Services RU-FU; 3211-08-000102, FU07-CT-2007-00065 Ministry of Education, Science and Sport
- Asst. Prof. Andrej Trkov
- 7FP EURATOM; Improvement of Diagnostic in Edge Plasmas of Fusion Devices 1.2.1.-FU; Annex 2 to Contract 3211-08-000102, FU07-CT-2007-00065 Ministry of Higher Education, Science and Technology Prof. Tomaž Gyergyek
- 7FP EURATOM; Neutronic Studies for DEMO 4.10.2. FU Ministry of Higher Education, Science and Technology Dr. Igor Lengar
- 7FP EURATOM, MHEST Association; Neutron Calculation for Fusion Reactor, JET MCNP Model - 3.4.1.-FU, TA JW12-FT-JET, JW12-NFT-MHST Ministry of Education, Science and Sport Dr. Igor Lengar
- EURATOM-MHEST, WP2013/3.4.3., 3.4.4., 3.4.5 Neutron Calculations for Fusion Reactor Ministry of Education, Science and Sport Dr. Igor Lengar
- 3.4.2-FU, EURATOM-MHEST, Neutron Calculations for Fusion Reactor-JET Neutron Source Calibration Ministry of Education, Science and Sport
 - Dr. Luka Snoj
- 12. 3.4.1-FU13, EURATOM-MHEST, JET MCNP Model Neutron Calculations for Fusion Reactor
- 13. Ministry of Education, Science and Sport Dr. Igor Lengar
- 7FP EURATOM-MHEST, WP12-SYS-02-T06-01/MESCS/PS, Tritium Breeding Ratio Assessment Minister of Education Science and Sport

Ministry of Education, Science and Sport Dr. Igor Lengar

- 7FP EURATOM-MHEST, Pref. Supp. WP13-IPH-A06-P1 -02/MESCS/PS, SOL Transport and Divertor Heath Loads in Steady State and Unmitigated ELMs Ministry of Education, Science and Sport Prof. Tomaž Gyergyek
- Feasibility Study and Installation of Thermal Neutron Driven 14 MeV Neutron Converter into the TRIGA Research Reactor IAEA - International Atomic Energy Agency
 - Dr. Luka Snoj
- Training and Tutoring for Experts of the NRAs and their TSOs for Developing and Strengthening their Regulatory and Technical Capabilities - INSC Project MC.03/10 -LOT 1: Training and Tutoring for Nuclear Regulatory Authorities and their TSO's ITER-consult Srl Dr. Luka Snoi

- Integral Measurements for the Validation of the Dosimetry Cross Sections; F41031 Testing and Improving the IAEA International Dosimetry Library for Fission and Fusion (IRDFF)
 - IAEA International Atomic Energy Agency Asst. Prof. Andrej Trkov
- IAEA Fellowship for Ms Widad Kouidri Titouche, ALG/10055, C6/ALG/10055, 15.04.-14.07.13
 - IAEA International Atomic Energy Agency Asst. Prof. Andrej Trkov
- Evaluation and Validation of the Resonance Parameters for Structural Materials Slovenian Research Agency Asst. Prof. Andrei Trkov
- Experimental Verification of Kinetic Parameters of the TRIGA Reactor and Upgrade of the Digital Meter of Reactivity Slovenian Research Agency
- Dr. Igor Lengar
- 22. Experimental Verification of Neutron Flux Form Factors and Qualification of a New Wide Range Multichannel Neutron Instrumentation Slovenian Research Agency
- Dr. Gašper Žerovnik 23. Design of Irradiation Device for FT-TIMS Method at the JSI TRIGA Mark II Reactor Slovenian Research Agency

RESEARCH PROGRAM

1. Reactor Physics Asst. Prof. Andrej Trkov

Dr. Luka Snoi

R&D GRANTS AND CONTRACTS

- Neutron Calculations for Use with Neutron Diagnostics Application to the JET Fusion Reactor Dr. Igor Lengar
- Functionalization of Biomedical Samples by Thermodynamic Non-equilibrium Gaseous Plasma
- Prof. Milan Čerček
 Calculations to Support Neutron Monitor Calibration JET Fusion Reactor Example Case Dr. Luka Snoj
- Determination of Computational Framework for Treating Gas Discharges in Case of Surge Protection Gas Discharge Tubes Dr. Jernei Kovačič
- Irradiation and Analysis of Si Samples Asst. Prof. Andrej Trkov

NEW CONTRACTS

- Reload Operational Core Analysis, Post Refueling Nuclear Design Check Tests, PIS and KFSS Cycle Specific Data for Future Fuel Cycles Krško Nuclear Power Plant Dr. Marian Kromar
- Expert Review of the Analysis and Testing Report for Capsule T for the Krško Reactor Vessel Irradiation Surveillance Program Krško Nuclear Power Plant
 - Dr. Marjan Kromar Development of Advanced Methods for the
- Development of Advanced Methods for the Description of Dynamic Processes in a Nuclear Reactor Krško Nuclear Power Plant

Asst. Prof. Andrej Trkov

VISITORS FROM ABROAD

- Dr. Roberto Capote Noy, International Atomic Energy Agency, Vienna, Austria, 31. 3.–8. 4. 2013
- Widad Kouidri Titouche, Commissariat a l'énergie atomique (COMENA), Centre de recherche nucléaire de Birine, Birine, Algeria, 14. 4.–13. 7. 2013
 Da Datziel Source da Francisco Orando Dispetencente de Inconsistent de Inconsistente de In
- Dr. Patrick Sauvan, dr. Francisco Ogando, Dipartamento de Ingenieria, Universidad National de Education a Distancia (UNED), Madrid, Spain, 8. 4.–12. 4. 2013
 Dr. Loic Barbot, dr. Damien Fourmentel, dr. Christian Jammes, CEA, Cadarache, France,
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STAFF

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- 1. Prof. Tomaž Gyergyek*
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- 11. Aljaž Čufar, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

- Jiři Adámek, M. Peterka, Tomaž Gyergyek, Pavel Kudrna, M. Ramisch, U. Stroth, J. Cavalier, Milan Tichy, "Application of the ball-pen probe in two low-temperature magnetised plasma devices and in torsatron TJ-K", In: 9th International Workshop on Electric Probes in Magnetized Plasmas, September 21-23, 2011, Iaşi, Romania, *Contrib. Plasma Phys.*, vol. 53, no. 1, pp. 39-44, 2013.
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DEPARTMENT OF EXPERIMENTAL PARTICLE PHYSICS F-9

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

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

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

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

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

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

ATLAS experiment

The amout of data delivered by the Large Hadron Collider (LHC) at CERN in 2011 and 2012 exceeded the most optimistic expectations and the analysis of the data is occupying the scientists of the ATLAS collaboration throughout 2013 as well as 2014. In addition to the analysis of the existing data the collaboration is preparing for the re-start of the Large Hadron Collider LHC in the year 2015, when it will begin to operate at the unprecedented centre-of-mass energy of 13 TeV.

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

The new particle, the discovery of which was announced at the seminar held on 4th of July 2012, was in 2013 confirmed to be the long-sought Higgs boson by measuring the particle properties (e.g., spin and parity). As a consequence of this discovery (Fig. 1) by the collaborations ATLAS and CMS the Nobel prize for Physics was in 2013 given for the theoretical prediction of the The discovery of the Higgs boson by the ATLAS and CMS collaborations is the reason for the Nobel Prize given for Physics in 2013.

Figure 1.: The 2013 European Physical Society's High Energy and Particle Physics Prize, for an outstanding contribution to high-energy physics was awarded to the ATLAS and CMS collaborations "For the discovery of a Higgs boson, as predicted by the Brout-Englert-Higgs mechanism". (From left) Joe Incandela, Peter Higgs, Francois Englert, Tejinder Virdee, Dave Charlton (ATLAS), and Peter Jenni (ATLAS).





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Figure 2.: Assembly of the new diamond detector DBM (Diamond Beam Monitor) of ATLAS. It will provide precise online measurements of the bunch luminosities at the LHC.

Higgs boson to P. Higgs and F. Englert and the prize itself cites the discovery of the Higgs boson by the ATLAS and CMS collaborations. The news about the discovery of the Higgs boson was published in practically all the world's media. This result is an important advance in our understanding of the basic forces holding the Universe together. In particular this new boson provides support for the existence of the proposed Higgs field, which explains how some particles come to have a mass and others do not. Without mass, all particles would fly around freely and matter as we know it would not exist. Physicists work to a theory of fundamental particles and their interactions called the Standard Model, which was first proposed in the 1970s. So far experiments have been able to confirm the existence of nearly all its elements with a high degree of precision. The Higgs boson, however, had eluded detection until now, prompting speculation that the theory could be incomplete. The findings so far suggest a Higgs boson compatible with the Standard Model, but further studies are needed to confirm this. We are looking for more Higgs particles, which according to almost all the high-energy extensions of the Standard Model, should exist. Some of the most popular new

models of physics are the so-called Super-symmetry theories, which could potentially solve a number of problems in theoretical physics. The most minimalist Super-symmetry theory predicts at least five (!) Higgs bosons: three neutral and two charged. So in the future, if we detect more than one, we will know that we are looking at a new physics. Searches for beyond-Standard-Model physics continued throughout 2013 and while a plethora of possible theories were statistically excluded, no discoveries of New Physics were as yet made. There are however good indications that such discoveries could be made when the LHC restarts in 2015 at the even higher energies.

A group of researchers from our department had one of the leading roles in the development, implementation and operation of two charged particle detector systems in the centre of the ATLAS spectrometer. Both systems, the Beam Conditions Monitor (BCM) and Beam Loss Monitor (BLM), are based on pCVD diamond sensors. The BCM is much more complex and has several functionalities. One task is monitoring the conditions of the LHC (Large Hadron Collider) proton beams at the interaction point in the centre of ATLAS spectrometer and issuing warnings at potential dangers. The BCM was the main luminosity monitor of the ATLAS experiment throughout most of the data-taking period of 2011 and 2012, when ATLAS was delivered about 30 fb-1 of data. In the second half of 2012 the BCM was enabled and was active in the Beam Interlock System and could have triggered a beam abort if the thresholds were reached.

The BLM is a much simpler system, the aim of which is the protection of the Inner Detector of ATLAS against potentially dangerous beam conditions. In summer 2011 the BLM twice triggered a LHC beam dump and prevented potential damage in the delicate silicon detectors of the Inner Detector.

Our group also developed and maintained the RADMON system that is used for recording the radiation doses due to charged particles and neutrons that different parts of the Inner Detector receive.

In 2013 the upgrade of the Large Hadron Collider started that will last for two years. During this period the LHC is being consolidated to be ready to operate at higher proton energy and higher luminosity. The ATLAS spectrometer is also being upgraded to be able to cope with a higher collision pileup. One of the most important upgrades is the

The Belle collaboration performed a series of measurements of rare processes that constrain the parameter space of several new physics models. Specifically, we measured parameters describing the difference between particles and antiparticles in processes with a significant quantum loops' contribution installation of an additional layer of silicon detectors for improved tracking and vertexing. A set of telescopes built on the basis of the same readout chip as used for the additional silicon layer and mostly using pCVD diamonds for the sensor material (Diamond Beam Monitor, DBM) is being installed and commissioned with a strong participation of the Ljubljana group. In 2013 the detectors were assembled, tested and installed into the final position in the centre of ATLAS. Currently, the works continue with a final connection and the development of firmware and software for the readout of data and the data acquisition.

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

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

One of the most interesting ways to find signals of the New Physics are decays in which a b quark from a B meson transforms into an s quark (as for example in the decay $B \rightarrow \eta' K_{c}$). This type of decay proceeds through the so-called "quantum fluctuations", where the b quark turns for very short period of time into a much heavier t quark and W boson, and then ends up as an s quark, together with a pair of a quark and an anti-quark. Instead of the t quark and the W boson new types of particles could show up in such a process that are not part of the Standard Model, and have not been discovered up to now. Such a hidden presence of new particles could change the values of the two parameters S and A of CP violation in the process under study, so that they would differ significantly from the values as determined in the decay $B \rightarrow I/\Psi K$, which cannot be influenced by quantum fluctuations. The experimental study of $B \rightarrow \eta' K_c$ (a topic of the PhD Thesis of Luka Šantelj) has shown (Figure 3) that the parameters of CP violation are consistent with the value of these two parameters in the decay $B \rightarrow J/\psi$ *K*. This means that while the effects of New Physics in this decay channel cannot be excluded, they must be quite small; this conclusion represents one of the most important results of the Belle Collaboration in 2013. Slovenian



Figure 3: CP violation measurement in $B \rightarrow \eta' K_s$ decays. Left: measured time evolution for B meson (blue) and antimeson (red) decays; the lower plot shows the time evolution of the asymmetry between the two decays. Right: measured value of the two CP violation parameters A and C (green) as compared to the world average in $B \rightarrow \eta'$ Ks decays (oval with a red boundary), previous Belle measurement (oval with a blue boudary) and with the value of both parameters as determined in the B $\rightarrow J/\psi$ Ks decays (chess board).

physicists have also led a study where a new method was developed and applied to measure for the first time the absolute probability of a decay of a charmed baryon Λ_c to a proton, a kaon and a pion. A precise value of this probability is required as an input in the interpretation of several other measurements, such as the exclusive and inclusive decay-rate measurements of b-flavored mesons and baryons or the measurements of fragmentation fractions of charm and bottom quarks. Another important result is a measurement of mixing in the system of neutral D mesons, as observed in the D meson decays into a kaon-pion pair.

In 2013, we continued with the preparation of the Belle II detector system. In this project, which includes almost 500 physicists from around the world, Slovenian colleagues play a key role, both in the management of the research group, as well as in developing new detection methods and methods for the analysis of the collected data.

Pierre Auger observatory

The Earth is exposed to a permanent rain of cosmic particles from outer space. Most of the particles are fully ionized atomic nuclei, moving with relativistic energies. The bulk of them with energies up to 10¹⁷ eV originate within our Milky Way. They are most likely accelerated in supernova remnants. Some particles have a thousand times higher energies, *i.e.*, around 10²⁰ eV. To clarify the origin of the highest-energy particles, their properties, like energy, arrival direction and the particle type (photons, protons, atomic nuclei), have to be measured. The highest-energy cosmic rays are extremely rare. On Earth one particle is registered in an area of 100 square kilometres in a hundred years. The measurement of such particles requires a huge measurement device that is operated for a long time.

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

Above 10° eV, the cosmic ray flux falls with energy E roughly as $E^{\gamma i}$ where the spectral index $\gamma \sim 3$. Several breaks in the spectral index have been observed, reflecting cosmic ray properties like the interaction between particles and the photons of the 3K microwave background at 4×10^{18} eV and a fall-off at energies exceeding 10^{19} eV due to cosmic acceleration processes being proportional to the magnetic field in the astrophysical sources. Due to growing statistics every year an updated measurement of the energy spectrum is published. At an exposure of 5400 km² × sr × year a suppression with $\gamma_1 = 2.59 \pm 0.02$, $\gamma_2 = 4.3 \pm 0.02$ and $\gamma_3 = 4.3 \pm 0.02$ was observed.

The identification of the type of the impinging cosmic-ray particle is experimentally the biggest challenge. Incoming particles such as atomic nuclei (of different masses), photons, and neutrinos induce cascades in the atmosphere. The longitudinal development of the showers depends on the particle type. Heavy nuclei interact early in the atmosphere, while light particles penetrate much deeper. This implies that for heavy nuclei the whole shower development takes place higher up in the atmosphere as compared to light particles. Thus, a measurement of the height of the shower above the ground is a good estimate for the mass of the primary particle. Technically, we measure the distance between the detector and the position at which the shower contains its maximum number of particles. The investigations indicate that cosmic rays are composed of light particles (such as protons and helium nuclei) at energies around 10^{18} eV. The data exhibit a trend towards heavier nuclei with increasing energy. At energies around 4×10^{19} eV, shower properties consistent with a heavy elemental composition (*e.g.*, silicon or iron nuclei) are observed. At higher energies, at present, no mass measurement is available due to the small flux of particles at such energies. These mass measurements do assume that we can correctly extrapolate hadronic physics from accelerator experiments.

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

Given that the highest energy cosmic rays observed should exhibit trajectories that are relatively unperturbed by galactic and intergalactic magnetic fields, it is natural to wonder whether isotropy begins to emerge at these high energies. Furthermore, if the observed flux suppression is the GZK effect, there is necessarily some distance, (100 Mpc), beyond which cosmic rays with energies near 10²⁰ eV would not be seen. Since the matter density within about 100 Mpc is not isotropic, this compounds the potential for anisotropy to emerge in the UHECR sample. The Auger Observatory provides two complementary approaches to determine the direction of an incoming cosmic ray. Stereo observations of the showers with multiple fluorescence telescopes provide a three-dimensional picture of the shower in the atmosphere and, thus, the orientation of the shower axis, pointing back into the direction of the incoming particle. Secondly, the measurement of the arrival times of the individual particles at the surface detectors allows us to measure the shower disc, with the arrival direction being perpendicular to it. Based on the Auger data set, 28 out of 84 events with energies higher than 5.6 x 1019 eV were found to be correlated with objects in the Veron-Cetty catalogue of active galactic nuclei. The overall correlation strength thus decreased from $62 \pm 10\%$ previously published to 33 ± 5%. However, the chance probability of observing such a correlation from a random distribution remains below 1%. Correlations on such a small angular scale as those reported (3.1°) would seem to be at odds with the apparent trend for a heavy composition at high energy, since heavier nuclei would be more deflected by intergalactic and galactic magnetic fields.

Distributed computing

SiGNET Tier-2 distributed computing site has increased its capacity to 2800 cores and 1200TB of data storage space in the year 2013. As a constitutive member of the Slovenian National Grid Initiative SLING/NGI the site had supported and maintained the Slovenian grid infrastructure together with Arnes. The Slovenian distributed infrastructure incorporates seven clusters from Jožef Stefan Institute, Arnes, Acrtur, University of Nova Gorica, and several others are in the process of joining, with a vision to create a powerful distributed computing infrastructure in Slovenia. The SiGNET is a full member of international organizations EGI/InSPIRE, wLCG and Nordugrid and had participated in several joint projects related to the support, maintenance and planning of the computing infrastructure as well as the development, distribution and deployment of the distributed computing infrastructure. It participated in education at several distributed computing workshops organized at Arnes and the Jožef Stefan



Figure 4: Silicon module assembled with direct bonding of the sensor to the circuit.

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

Detector development

In 2013, we continued with the development of new methods for the detection of annihilation gamma rays in positron emission tomography (PET), one of the most important medical imaging methods. If a Cherenkov radiator is used as a gamma-ray converter instead of a scintillator, the difference in the time of flight of the two gamma rays can be measured with a very high precision of 80ps (FWHM). In this way we can directly obtain three-dimensional information on the emission point of the two gamma rays, which substantially reduces the time needed to determine the activity distribution in the patient [4]. We have also developed a new method for the detection of gamma rays with a scintillator in which the depth of the gamma-ray conversion within the crystal is determined from a ratio of signal

intensities in the neighbouring detector pixels. In 2013, a review article on photon detection was published Annual Review of Nuclear and Particle Science.

We developed a rigid flex circuit bound with a compact silicon sensor (by Hamamatsu Photonics) and readout electronics (by IDEAS, Oslo). The design of the circuit and the binding procedure were developed at our department within the Research Voucher program on behalf of the Elgoline, d.o.o. company from Cerknica (Fig. 4). Measurements with a calibration 241-Am radioactive source showed that the innovative binding scheme had no effect on the system performance. Such a scheme can be critical in applications where the dense packing of detectors is required as in a setup to measure the interactions of gamma rays in nuclear medicine

In 2011 and 2012 we collected a substantial collection of PET probe data, which offers the possibility to study the effects of the spatial resolution of the sensors on the image quality. For a precise analysis a physical model of the image generation procedure had to be developed along with a model-based reconstruction method of the collected data. With data from the collection we were able to confirm the model validity and the model will be used in the planning of new imaging methods and their impact on diagnostic procedures and treatment.

Development of radiation hard silicon detectors is very important for future high-energy experiments. We used an innovative edge-TCT method, developed at our laboratory, to measure the electric field in silicon detectors. The detectors were irradiated at nuclear reactor in Podgorica near Ljubljana with neutrons up to fluences of 5×10^{16} cm². Sensors with slim edges allow dense packing with a small loss of efficiency. The efficiencies of sensors with SCP (Scribe Cleave Passivate) edges were measured with laser light

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

Organization of conferences, congresses and meetings

1. Meeting of users and administrators and network computing of Slovenian network for national GRID infrastructure, Jožef Stefan Institute, Reactor Center in Podgorica, Podgorica, Slovenia, 13. 11. 2013

INTERNATIONAL PROJECTS

- Design, Procurement and QA of Flex-rigid Hybrids European Organization for Nuclear Research Prof. Marko Mikuž
- 2. 7FP EGI-InSPIRE; European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe European Commission
- Prof. Marko Mikuž
- 7FP AIDA; Advanced European Infrastructures for Detectors at Accelerators European Commission Prof. Marko Mikuž
- 7FP HadronPhysics3; Study of Strongly Interacting Matter European Commission
- Prof. Samo Korpar
- FERRO-PATCH; Frequency and Polarisation Agile Microstrip Patch Antenna based on Ferrelectric Varactors
- ESA/ESTEC.
- Prof. Vladimir Cindro 6. Development of Silicon and Diamond Semiconductor Detectors for Particle Physics
- Experiments and Medical Imaging Slovenian Research Agency
- Dr. Andrej Gorišek
- Doping of Semiconductor Nanocrystals by Neutron Transmutation Method (NTD) Slovenian Research Agency Asst. Prof. Igor Mandić
- Evaluation of the Prototype of a Double-ring PET Device Slovenian Research Agency Prof. Marko Mikuž
- Development and Tests of a Method for Particle Identification with a TOP Counter Slovenian Research Agency Prof. Marko Starič
- 101 Mathods and Accuracies of the Mixing and CP Violation Measurements of the Charmed Hadrons at the Belle II Experiment Slovenian Research Agency

Prof. Boštjan Golob

RESEARCH PROGRAMS

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

R&D GRANTS AND CONTRACTS

- 1. ATLAS Diamond Beam Monitor Prof. Marko Mikuž
- Search for Microscopic Black Hole Signatures with Ultra-high Energy Cosmic Rays Prof. Marko Zavrtanik
 - Development of Solid State Detectors for Particle Physics Experiments
- 4. Prof. Vladimir Cindro

3.

- Novel Detection Methods based on Cherenkov Radiation Prof. Peter Križan
- Development of In-vivo Dosimetry for Applications in Radiotherapy Dr. Gregor Kramberger
- Measurement of the Absolute Branching Fractions of Leptonic D(s) Decays and the Extraction of the Decay Constant f_D(s) Dr. Anže Zupanc
- Collaboration CERN RD-39
- Prof. Marko Mikuž
- Collaboration CERN RD-50 Prof. Marko Mikuž
- 10. Collaboration DELPHI
- Prof. Borut Paul Kerševan
- 11. Collaboration ATLAS
- Prof. Marko Mikuž 12. Collaboration CERN RD-42
- Prof. Marko Mikuž
- 13. Collaborations Belle in Belle II
- Prof. Peter Križan
- 14. Collaboration CIMA; Cameras for Imaging in Medical Applications Prof. Marko Mikuž



NEW CONTRACTS

- Reliability Investigation of High Density Interconnect Circuits INTEC TIV, d. o. o. Prof. Vladimir Cindro
- 2. Data-Storage System

Xenya, d. o. o. Prof. Andrej Filipčič

VISITORS FROM ABROAD

- 1. Dr. Christian Joran, CERN, Genève, Switzerland, 1. 1.-10. 1. 2013
- 2. Dr. Ivana Capan, Institut Ruđer Bošković, Zagreb, Croatia, 4. 4.-6. 4. 2013

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- 8. Dr. Gregor Kramberger
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- 16. Prof. Danilo Zavrtanik*
- 17. Asst. Prof. Dejan Žontar*

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- 18. Dr. Matej Batič, left 01.03.13
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- 3. Prof. Dr. Neal C. Clinthorne, University of Michigan, USA, 19. 5.-23. 5. 2013
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- 21. Jyoti Prakash Biswal, B. Sc.
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- 30. Aleš Svetek. M. Sc.
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- 32. Tina Šfiligoj, B. Sc
- 33. Elvedin Tahirović, B. Sc.
- 34. Dr. Andrii Tykhonov, left 01.10.13
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- 36. Jurij Eržen
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ORIGINAL ARTICLE

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momentum at $\sqrt{s} = 7$ TeV with the ATLAS detector", *Phys. lett., Sect. B*, vol. 720, no. 1/3, pp. 32-51, 2013.

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- 14. ATLAS Collaboration, G. Aad *et al.*, "Measurement of the inclusive jet cross-section in *pp* collisions at $\sqrt{s} = 2.76$ TeV and comparison to the
- 15. ATLAS Collaboration, G. Aad *et al.*, "Measurement of the jet radius and transverse momentum dependence of inclusive jet suppression in leadlead collisions at $\sqrt{S_{NN}} = 2.76$ TeV with the ATLAS detector", *Phys. lett., Sect. B*, vol. 719, no. 4/5, pp. 220-241, 2013.
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- 23. ATLAS Collaboration, G. Aad *et al.*, "Search for direct chargino production in anomaly-mediated supersymmetry breaking models based on a disappearing-track signature in *pp* collisions at \sqrt{s} = 7 TeV with the ATLAS detector", *J. high energy phys.*, vol. 2013, no. 1, pp. 131-1-131-34, 2013.
- 24. ATLAS Collaboration, G. Aad *et al.*, "Search for direct production of charginos and neutralinos in events with three leptons and missing transverse momentum in $\sqrt{s} = 7$ TeV *pp* collisions with the ATLAS detector", *Phys. lett., Sect. B*, vol. 718, no. 2, pp. 841-859, 2013.
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- 65. ATLAS Collaboration, G. Aad *et al.*, "Search for long-lived stopped *R*-hadrons decaying out of time with *pp* collisions using the ATLAS detector", *Phys. rev., D Part. fields gravit. cosmol.*, vol. 88, no. 11, pp. 112003-1-112003-30, 2013.
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INDEPENDENT COMPONENT PART OR A CHAPTER IN A

Monograph

- 1. Andrej Studen, "Image magnification with PET insert probe", In: *Imaging in nuclear medicine*, Augusto Giussani, ed., Christoph Hoeschen, ed., Berlin, New York, Springer, cop. 2013, pp. 203-222.
- Andrej Studen, "Physics of imaging in nuclear medicine", In: *Imaging in nuclear medicine*, Augusto Giussani, ed., Christoph Hoeschen, ed., Berlin, New York, Springer, cop. 2013, pp. 19-41.

MENTORING

- 1. Milan Grkovski, *Development of a high resolution PET probe:* doctoral dissertation, Ljubljana, 2013 (mentor Dejan Žontar).
- 2. Andrej Seljak, *Proximity focusing RICH with aerogel as radiator:* doctoral dissertation, Ljubljana, 2013 (mentor Samo Korpar).
- Peter Smerkol, Measurement of CP violation parameter A_{CP} in weak decays of charmed baryons Λ_C with the Belle detector: doctoral dissertation, Ljubljana, 2013 (mentor Boštjan Golob).
- 4. Luka Šantelj, Measurement of time-dependent CP violation in $B \rightarrow \eta' K_s^0$ decays: doctoral dissertation, Ljubljana, 2013 (mentor Boštjan Golob).
- 5. Andrii Tykhonov, *Searches for dark matter and lepton-jets with the ATLAS detector:* doctoral dissertation, Ljubljana, 2013 (mentor Borut Paul Kerševan).
- 6. Tara Nanut, Študij vpliva ozadja na meritev razpadov $D^+ \rightarrow \pi^+ l^+ l^- z$ detektorjem Belle: master's thesis, Ljubljana, 2013 (mentor Boštjan Golob).

DEPARTMENT OF INORGANIC CHEMISTRY AND TECHNOLOGY K-1

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

In the research field of new inorganic compounds the study of the VOF, reactivity towards different fluoride Lewis bases was continued. The reaction of VOF₂ with SeF₄ yields SeF₄ [$V_2O_3F_7$]. Xenon fluorides reacted with VOF₂ according to their basicity. The Lewis acid-base adduct XeF, VOF, was isolated in the XeF, system, while the reaction with XeF_6 led to the formation of $XeF_5[VOF_4]$ salt. XeF_4 as a weaker base does not form any kind of product with Head: VOF₃. XeF₂ as a ligand to a metal centre was studied over the past decade and a whole series of compounds was Asst. Prof. Gašper Tavčar prepared. One of the latest examples is $[Ca_2(XeF_2)_2][NbF_6]_6$, in which the are three different calcium centres with completely different coordination spheres. The numbers of XeF, molecules connected to calcium atoms are four, three and even one. Fluorine atoms from NbF₆ units complete the coordination sphere.



During the investigation of reactions between alkaline metal fluorides and titanium tetrafluoride in an anhydrous hydrogen fluoride solvent, single crystals of K₄Ti_eF_{4c}.8HF and Rb₄Ti_eF_{4c}.6HF were prepared and their

crystal structures determined. Both structures contain previously unknown discrete octameric $[Ti_8F_{36}]^{4-}$ anions. Each of them is constructed from eight TiF₆ octahedral units sharing joint vertices and connected in that way into a cube. The herein reported $[Ti_{8}F_{36}]^{4-}$ anion represents the largest known example of discrete oligomeric species found in fluoride compounds with the metal in the oxidation state four.

Anion [Ti₈F₃₆]⁴⁻ represents the largest known example of discrete oligomeric species found in fluoride compounds with a metal in oxidation state four.

The compounds H₀[Ti_.F_.], H₀[SnF.], (H_.0), [SnF.] and Na(HF)[Sn.F_.] were successfully synthetized and characterized. The structure of Na(HF)[Sn,F,] reveals a rare example of HF acting as a ligand towards sodium centres and simultaneously interacting through hydrogen bonding with the double chain of the polymeric anion $([Sn_{2}F_{0}]^{-})_{m}$. Until now, the description of the aforementioned anion was based only on data obtained from spectroscopic measurements.

In cooperation with the University of Warsaw (Poland), IMCN (Université Catholique de Louvain) and the University in Ljubljana (FCGE) we have investigated the magnetic and structural properties of potassium trifluoridoargentate(II). The results of the magnetic studies show strong super-exchange antiferromagnetic interactions between neighbouring silver(II) ions within the chains. The strength of the interactions is reminiscent of that found in superconductors based on copper(II) oxides.

The syntheses of copper(I) salts p-complexes with functional derivatives of selected organic compounds were performed, and the obtained products were characterized. Crystalline copper(I) ω-complexes with fluorine containing anions $[Cu(L)CF_2SO_2]$ and $[Cu_2(L)_2(H_2O)_2](SiF_2)_2 \cdot 2.5H_2O(L - 2-(allyl)$ amino-5-methyl-1,3,4-thiadiazole) have been obtained by an electrochemical technique and investigated. The organic molecule L acts as a chelate-bridging tridentate ligand, connected to copper(I) by two N atoms of a thiadiazole ring and a C=C bond from the allyl group resulting in the formation of stable cationic dimers $[{Cu(L)}_{2}]^{2+}$. The direct synthesis of coordination compounds from a mixture Cu-DMSO-CCl₄-ligand has been explored. A unique bridging mode of the DMSO molecule in the compound 2CuCN·DMSO was observed. DMSO is bonded to two Cu⁺ centres *via* oxygen and sulphur atoms.



Figure 1: Coordination sphere of sodium atoms and bonding of HF molecules in the structure of Na(HF)[Sn2F9]

New catalytically active transition-metal sulphides-based nanomaterials are especially effective in the hydrodeoxygenation of liquefied biomass.

Ions containing solely fluorine atoms, F⁻, F₂⁻ and F₃⁻ and their corresponding cationic and/or multiply charged counterparts were investigated. The emphasis has been put on gas-phase species. A linear relationship between the entropy of formation of aqueous anions and the independent simple parameters derived from the ionic stoichiometry of the species has been derived. In comparison with previous equations, newly derived equa-

tions are based on a smaller set of parameters and enable the calculations of entropies of formation of unknown anions with a precision and accuracy comparable to earlier equations.

Possibilities for the direct preparation of fluoride aerogels were further investigated. Work in this field was focused on the determination of the main solvothermal conditions that lead to the formation of aerogels based on



Figure 2: Comparison of the structure of KAgF₃ with structures of oxocuprates(II) and iron(III) based superconductors (back cover of the journal Chem. Comm. 49 (2013), 6262-6264)

aluminium(III) fluoride, AlF₂. It was found that very open and voluminous aerogel structures are obtained only when methanol is one of the applied non-aqueous solvents, and when the drying of the precursor sols or gels is performed at supercritical conditions. Products from such preparations consisted of elongated and partially crystallised fluoride nanoparticles with remarkably uniform shapes and dimensions. The crystal structure perfectly corresponded to β-AlF₂, although the determined composition, AlF₂ (OH) yH,0 (0<x<0,2), indicated a partial F⁻ for HO⁻ ion exchange, which can be associated with partial hydrolysis. In systems containing methanol, the formation of thermally and chemically very stable surface methoxide groups was observed. These groups apparently favour the formation of elongated particles and prevent their agglomeration, and, simultaneously, block the surface Lewis acid sites, which is reflected in the strongly reduced catalytic activity. The importance of these investigations is not solely in the addition of a new class of materials to the group of so-called "exotic" aerogels, but also in the established capability of the method for the preparation of fluoride nanoparticles with well-defined sizes and shapes. Fluorides with such characteristics cannot be obtained by conventional synthetic approaches.

The economic utilization of liquefied wood as a fuel is inhibited by its high oxygen content. However, with the catalytic hydrodeoxygenation (HDO) process the oxygen content in liquefied wood can be lowered to such an extent that processed liquefied wood becomes a competitive fuel. New catalytically active transition-metal sulphides based nanomaterials were prepared and are especially effective in fuel production HDO reactions and represent a



Figure 3: Acta Chimica Slovenica, Issue No. 3, 2013, was dedicated to prof. Boris Žemva on the occasion of his receiving the Zois Award for lifetime achievements in the field of inorganic fluorine chemistry (Design cover: KULT, oblikovalski studio, Simon Kajtna s.p.)

low-cost alternative to noble-metal-based catalysts. The research work was done in cooperation with the National Institute of Chemistry, Slovenia.

In the EU FP7 project Integ-Risk we continued our work on methods and tools for the management of new and emerging risks in industry. In that respect we tested in the industrial zone of Luka Koper (Port of Koper), Slovenia and in the Industrial Zone Pančevo, Serbia, methods for: i.) analysing the risks between the client and contractors, ii.) an approach to the selection of the key performance indicators (applied to the process safety), iii.) an approach to the analysis of energy-supply security, iv.) an approach to the assessment of the health effects due to exposure to hazardous substances, v.) the domino accident potential among two industrial establishments, vi.) a tool for the spatial integration of the risk information (process safety aspect) and vii.) an approach to consider the risk information within the process of land use planning/plan elaboration (at the local community level). In 2013 we mainly reported about the work done on the final project meetings and submitted reports.

We continued work within EU COST action ES 1006 - Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments. Within the action we participate in the assessment of the accuracy of the existing hazardous substances atmospheric dispersion models into the ambient air in a complex/urban environment, as well as in the preparation of the best-practice guideline for the selection, modelling, use and interpretation of the results, including real-time support to the emergency response team managers.

In 2013 we started a new EU 7FP project TOSCA (Total Operations Management for Safety Critical Activities) in which we participate as a partner. The project deals with the integration of the individual management aspects industrial operations as a total safety, quality and productivity management system (at the company level), covering the whole life cycle of the product. In the project we participate during the definition of industrial needs (with a special emphasis on the SME

companies), the development and integration of the TOSCA methods and tools, the demonstration and validation of the proposed methods and tools for the industrial partners (also from Slovenia) and during the evaluation, standardization and dissemination of the project results.

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

The IPA project Adriacold "Diffusion of cooling and refreshing technologies using the solar energy resource in the Adriatic regions", started in October 2012, was continued in 2013 with partners from Italy, Slovenia, Croatia, Bosnia & Herzegovina and Albania. The JSI leads the Work Task "Monitoring and data mining", which comprises the planning and systematic collection of performance data for six pilot and testing cooling plants (in the cities of Dubrovnik and Rijeka (Croatia), Piran (Slovenia), Bazovica, Rimini and Bari (Italy)), and data analysis. Within the Work Task 4 "Installation of pilot and demonstration plants" we developed, along with Slovenian industry, which



Figure 4: SEM image of a MoS, catalyst (foto: Gleb Veryasov)

designs and markets such equipment, basic and minimal requirements for the monitoring equipment, needed for an effective evaluation of the cooling equipment efficiency. These requirements are one of the inputs for the tenders for the installation and operation of sustainable cooling devices. The requirements include sensor quality specifications and requirements for the safe storage and communication of the operational data.

By joining in the EMILIE project (Enhancing Mediterranean Initiatives Leading Innovation and SMEs to building Energy Efficiency Technologies) in 2013, carried out as part of the transnational cooperation program in the Mediterranean region, we became one of the members of the group of six research institutions to test and disseminate knowledge on innovative and competing technologies, products and solutions in the field of energy efficiency in buildings. The purpose of the 30-month project is to provide support to small and medium-sized enterprises in the

development, deployment and use of energy efficient technologies, thus contributing to strengthening the competitiveness and innovation of their products and processes. Within the project, the Institute is preparing a larger demonstration pilot facility, with several built-in innovative solar thermal technologies and systems for the use of waste heat. It will serve for the assessment, display and promotion of the concept of a new infrastructural economic model, which would allow greater use of solar energy and cost reduction for end-users in the tertiary sector.

We successfully concluded our work within the EU 7FP project iNTeg-Risk. One of the important goals of the project was the development, integration and demonstration of the proposed solutions for analysing and the management of emerging risks to society and industry.

The work within the project "Methodology of fixation of CO_2 on fly ash" was continued along with the partners from the Razvojni center Energija d.o.o. (RCE) (Development Centre Energy d.o.o.), where the department researchers provide consulting and support work for technology development on the pilot and semi-industrial scale based on laboratory-test findings. The process scheme was developed and the laboratory plant constructed, which was used for optimisation of the self-designed gas injection nozzles and a successful 48-hour test was performed, followed by a 48-hour semi-industrial test at the premises of the partner company Esotech in Velenje.

The activity in the field of education and the promotion of sciences should be mentioned. Five co-workers were actively engaged in the work of the Jožef Stefan International Postgraduate School as lecturers and as mentors to M.Sc. and Ph.D. students. In addition, the School of Experimental Chemistry maintained its very important relations with elementary, secondary schools and even kindergartens through experimental courses performed in a specialised laboratory or through direct demonstrations at the schools. With demonstrations of chemical experiments we participated at the 19th Slovenian Science Festival, organized by the Slovenian Science Foundation and at the Researchers night in Ljubljana.

In the past year, we successfully completed the European project KidsINNscience, in which we have systematically gathered innovative practices in science education from each of the partner countries. We have a collection of 80 teaching practices for different levels of education. A total of 28 innovative practices were selected for transfer to educational institutions. Good innovative teaching practice helps to increase motivation and

Figure 5: Innovative practice Cooking with the Sun originated from Spain. Students tried to build improvised devices, appropriate for cooking in a small bowl (foto: Matevž Kramer).

reduce disparities among students (boys/girls, children with special needs, etc.). It should be described clearly enough, but be flexible enough so that it can be used in different environments. Eight European countries: Austria (coordinator), Italy, Germany, the Netherlands, Spain, Switzerland, Great Britain and Slovenia, and two others, Brazil and Mexico, participated in the project.

Some outstanding publications in 2013

- Shlyapnikov, I., Goreshnik, E. A., Mazej, Z.: The cubic [Ti₈F₃₆]⁴ anion found in the crystal structures of K₄Ti₈F₃₆/8HF and Rb₄Ti₈F₃₆·6HF, Chem. Comm., 49 (2013), 2703–2705
- 2. Tavčar, G., Žemva, B.: $[Li(XeF_2)_n](AF_6)$ (A = P, As, Ru, Ir), the first xenon(II) compounds of lithium, Synthesis, Raman spectrum and crystal structure of $[Li(XeF_2)_3](AsF_6)$, Inorg. Chem., 52 (2013), 4319–4323
- 3. Kurzydłowski, D., Mazej, Z., Jagličić, Z., Filinchuk, Y., Grochala, W.: Structural transition and unusually strong antiferromagnetic superexchange coupling in perovskite KAgF₂, Chem. Comm., 49 (2013), 6262–6264
- 4. Shlyapnikov, I., Mercier, H. P. A., Goreshnik, E. A., Schrobilgen, G. J., Mazej, Z.: Crystal structures and Raman spectra of imidazolium poly[perfluorotitanate(IV)] salts containing the [TiF₉]², ([Ti₂F₉])_∞, and [Ti₂F₁₁]³ and the new [Ti₄F₂₀]⁴ and [Ti₅F₂₃]³ anions, Inorg. Chem., 52 (2013), 8315–8326
- 5. Stergaršek, A., Horvat, M., Frkal, P., Ribeiro Guevara, S., Kocjančič, R.: Removal of Hg⁰ in wet FGD by catalytic oxidation with air A contribution to the development of a process chemical model, Fuel, 107 (2013), 183–191

Patent granted

- 1. Andrej Kovič, Adolf Jesih, Aleš Mrzel, The procedure for the synthesis of 4d and 5d (Nb, Mo Ta, W) nitrites of transition metals in the form of quasi-one-dimensional structures, SI23988 (A), Urad RS za intelektualno lastnino, 30.8.2013.
- Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih, Procedure for synthesis of threadlike tungsten oxide W5014, US8496907 (B2), US Patent Office, 30.7.2013.

INTERNATIONAL PROJECTS

- 1. Export of the Fluorinated Carbons Foreign Clients Dr. Zoran Mazej
- Zofan Maxy
 7FP iNTeg-Risk; Early Recognition, Monitoring and Integrated Management of Emerging, New Technology Related Risks European Commission
- Asst. Prof. Marko Gerbec
- 7FP KidsINNscience; Innovation in Science Education Turning Kids on to Science European Commission Tomaž Ogrin, M. Sc.
- 7FP TOSCA; Total Operations Management for Safety Critical Activities European Commission
- Asst. Prof. Marko Gerbec
 IPA ADRIATIC; ADRIACOLD Diffusion of Cooling and Refresing Technologies using the Solar Energy resources in the Adriatic Regions Consorzio per L'Area di Ricerca Scientifica
- Asst. Prof. Gašper Tavčar

 MED - EMILLE; Enhancing Mediterranean Initiatives Leading SMEs to Innovation in Building Energy Efficiency Technologies Joint Technical Secretariat Med Programme Asst. Prof. Gašper Tavčar

 COST ES1006; Evaluation, Improvement and Guidance for the Use of Local-scale Emergency Prediction and Response Tools for Airborne Hazards in Built Environments COST Office Asst. Prof. Marko Gerbec.

 IPA ADRIATIC; ADRIACOLD - Diffusion of Cooling and Refresing Technologies Using the Solar Energy Resources in the Adriatic Regions Ministry of Economic Development and Technology Asst. Prof. Gašper Tavčar

Asset From Casper Farcar Programmer and Carbons by Phosphoric Acid Activation and their Application for Heavy Metal Removal and Improvement of Transition Metal Catalysts Slovenian Research Agency Dr. Adolf Iesih

RESEARCH PROGRAM

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

R&D GRANTS AND CONTRACTS

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

NEW CONTRACT

1. Fly ash CO2 Fixation Methodology RCE - Research Centre Energy, d. o. o. Dr. Robert Kocjančič

VISITOR FROM ABROAD

 Prof. Natalia Sikh, Valentyna Volynets, Institute for Sorption and Problems of Endoecology, NAS Ukraine, Kiev, Ukraine, 7. 10.–14. 10. 2013

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- 1. Asst. Prof. Marko Gerbec
- 2. Asst. Prof. Evgeny Goreshnik
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- 18. Peter Frkal, M. Sc. 19. Tine Oblak, M. Sc.
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- 21. Pero Kolobarić
- 22. Robert Moravec
- 23. Mira Zupančič

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- 12. Igor Shlyapnikov, Hélène P. A. Mercier, Evgeny A. Goreshnik, Gary J. Schrobilgen, Zoran Mazej, "Crystal structures and Raman spectra of imidazolium poly[perfluorotitanate(IV)] salts containing the [TiF₆]²⁻, ([Ti₂F₉]⁻)∞, and [Ti₂F₁₁]³⁻ and the new [Ti₄F⁴⁻₂₀ and [Ti₅F³⁻₂₃ anions", *Inorg. chem.*, vol. 52, no. 15, pp. 8315-8326, 2013.

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- 1. Norbert Chilingarov, Igor Shlyapnikov, Zoran Mazej, A. E. Moiseev, Y. M. Shliapnikov, I. V. Ishtubaev, "The study of cerium tetrafluoride vaporization by Knudsen effusion mass spectrometry", In: *Workshop on Knudsen Effusion Mass Spectrometry, April 23-25, 2012, Juelich, Germany,* (ECS transactions, Vol. 46, 1, 2013), Pennington, Electrochemical Society, 2013, vol. 46, no. 1, pp. 191-195, 2013.
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INDEPENDENT COMPONENT PART OR A CHAPTER IN A

MONOGRAPH

1. Erhard Kemnitz, Tomaž Skapin, John M. Winfield, "Preperation of fluorinated γ-alimina", In: *Efficient preparations of fluorine compounds*, Herbert W. Roesky, ed., Hoboken, Wiley, 2013, pp. 442-447.

PATENT APPLICATION

1. Adolf Jesih, Andrej Kovič, Aleš Mrzel, *Method for a synthesis of quasi one-dimensional structures of 4D and 5 D (Nb, Mo, Ta, W) transition metals*, W02012177224 (A3), World Intellectual property organization, 21.2.2013.

PATENT

- 1. Andrej Kovič, Adolf Jesih, Aleš Mrzel, *The procedure for the synthesis of* 4d and 5d (Nb, Mo Ta, W) nitrites of transition metals in the form of quasi-one-dimensional structures, S123988 (A), Urad RS za intelektualno lastnino, 30.8.2013.
- 2. Maja Remškar, Marko Viršek, Miha Kocmur, Adolf Jesih, *Procedure for* synthesis of threadlike tungsten oxide W_5O_{14} , US8496907 (B2), US Patent Office, 30.7.2013.

MENTORING

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- Peter Frkal, Removal of mercury from flue gas in wet desulphurization process: master's thesis, Ljubljana, 2013 (mentor Marko Gerbec; comentor Milena Horvat).

DEPARTMENT OF PHYSICAL AND ORGANIC CHEMISTRY K-3

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

Experimental research in the field of electrochemistry is oriented to various types of corrosion protection – from surface layers to functional modifications of the surface and corrosion inhibitors. The materials of interest are used in technological and biomedical applications. Within the project Surfuncti financed by the European Research Area (ERA) we have investigated a novel alloy for the biomedical applications, Ti-20Nb-10Zr-5Ta. This alloy exhibits better mechanical properties, i.e., a lower elastic modulus and higher hardness, than commercial titanium alloys. At the same time it is more corrosion protective under simulated physiological conditions. The composition of the layer changes depending on the potential and contains sub-oxides and oxides of all the alloy components. At more negative potentials the layer contains a mixture of sub-oxides (Ti2O3, NbO/NbO2, TaO/TaO2) and oxides (TiO2, Head: Nb,O, ZrO, Ta,O,), with titanium oxide being the predominant oxide. With the increasing electrode potential the **Prof. Ingrid Milošev** content of sub-oxides decreases and the highest valence oxide prevails. Compared to other elements, the oxidation of tantalum is inhibited. While other alloying elements are almost completely transformed to the highest valence

oxide, i.e., TiO₂, Nb₂O₅ and ZrO₂, tantalum remains mainly in the metal and sub-oxide, TaÕ/TaÕ,, forms. Thus, the formation of the pentoxide ${\rm Ta}_2{\rm O}_5$ as the highest valence oxide is suppressed compared to the oxides of other alloying elements. Metal cations of alloying components in the form of oxides are enriched in the layer relative to the metal content in the bulk alloy. It is hypothesized that this is the main reason for the exceptional protectiveness of the passive layer formed on the Ti-20Nb-10Zr-5Ta alloy. The long-term effects of an alloy implanted in the recipient's body were investigated in a minimum essential medium (MEM), using two types of human cells - an osteoblast-like cell line (HOS) and immortalized pulmonary fibroblasts (Wi-38). In terms of biocompatibility, the novel alloy performs similar to titanium. The project was performed in collaboration with the Institute of Physical Chemistry "Ilie Murgulescu" from Bucharest and the Faculty of Health Sciences University of Primorska.

The research also continued on commercial biomedical alloys. The formation of the oxide layer on Ti-based materials - Ti metal and Ti-6Al-7Nb and NiTi alloys - in acetic acid was studied at two potentials of interest, 0.7 V and 3.0 V. Regardless of the substrate, the main oxide component formed was titanium(IV) oxide, TiO2. The layer formed on the Ti-6Al-7Nb alloy contained oxides of minor elements, Al₂O₂ and Nb₂O₅, while the layer formed on Nitinol contained a small amount of nickel. The composition of the oxide layer is similar on all three substrates, but its thickness differs according to the oxidation potential and type of substrate. The thickness increases in the following order as a function of substrate: NiTi < Ti-6Al-7Nb < Ti. Anodization in acetic acid, and the resulting formation of TiO₂ at the substrate, beneficially affects the corrosion behavior of all three materials in a simulated physiological solution. Similar treatment, i.e., anodic oxidation in sodium hydroxide, was used for the corrosion protection of biodegradable magnesium alloys. The corrosion rate of this material is so high that its degradation may occur before the end of the healing process. An oxide film formed by anodic oxidation reduced the corrosion rate and slowed down the dissolution of magnesium, as proved by complexometric titration.

Metallic materials used for the manufacture of dental implants have to exhibit a high corrosion resistance in order to prevent metal release. A new hybrid coating for the corrosion protection of metals in various corrosive media was developed. This coating is an alternative to the traditionally most successfully used chromate coatings; their use is today restricted due to toxicity and carcinogenicity. This achievement was included in the international programme Bastille LCC and resulted in a patent application filed in the USA in 2013.



Figure 1: Various types of corrosion protection developed in our laboratory: (a) formation of a protection anodic layer on a magnesium alloy by anodic oxidation in NaOH, (b) synthesis of hybrid sol-gel coating on an aluminium alloy, (c) formation of conversion coating based on lanthanum nitrate on the intermetallics on aluminium alloy, and (d) formation of self-assembled layer of stearic acid on copper.



Figure 2: Adsorption configuration (a) and normalized histograms of atomic positions relative to Cu(111) surface (b) for cysteine molecule in an acid medium. In insets the medium is excluded to present more clearly the adsorption configurations of the molecules at the Cu(111)surface (turquoise). Legend: amino acid: O(red), N(blue), S(yellow), C(green), H(grey); medium: $H_2O(white)$, $H_3O^+(red)$, Cl(green).

The oral cavity is aggressive towards metals as it represents a multivariate environment with a wide range of conditions, including temperature, pH, the presence of bacteria and the effect of abrasion. An increasing use of various Ti-based materials for dental implants and orthodontic brackets poses the question of their corrosion resistance in the presence of fluoride ions, which are added to toothpaste and mouth rinse. The corrosion behaviour of Ti metal, Ti-6Al-7Nb and Ti-6Al-4V alloys investigated in artificial saliva was significantly affected by the presence of fluoride ions. The layer formed was less protective than that formed in a fluoride-free solution. At the surface, calcium fluoride and/or sodium and potassium hexafluorotitanate and hexafluoroaluminate were formed.

Among materials important for use in industry we have studied the corrosion protection of alloys based on aluminium, copper and zinc. The formation of various coatings on the surface of metals and alloys is one way of corrosion protection for technologically important materials. Due to their

beneficial properties aluminium and its alloys are used in numerous applications in civil engineering, automotive and aerospace industry, food and electronic industry. These materials exhibit low density, high tensile strength, excellent thermal and electrical conductivity and high strength-to-weight ratio. For many decades the chromate coatings represented the most effective corrosion protection of aluminium alloys. Since their production implies

Our co-worker dr. A. Kokalj is ranked as the most cited scientist in the field of Chemistry (source: SICRIS). Among the top twenty most cited authors, there are three co-workers from our department. the use of toxic compounds, the use of chromate coatings was banned or restricted in 2002 by European regulations. Today, new alternatives for chromate coatings are investigated, which would achieve comparable corrosion protection while being environmentally acceptable. In that context the development of sol-gel coatings is important. In our laboratory we are devoted to the development of hybrid sol-gel coatings that enable effective corrosion protection of aluminium and its alloys (AA2024 and AA7075). Hybrid coatings developed in the laboratory were awarded as best innovative

project at the Sixth International Technology Transfer Conference & Innovation Day 2013. This innovation was included in programme Bastille LCC and the patent application was filed in the USA.

Lanthanoid salts are also considered as a potential replacement for toxic and carcinogenic chromate coatings. The effectiveness of inhibition increases in the following order: $CeCl_3$, $La(NO_3)_3$, $LaCl_3$, $Ce(NO_3)_3$ in $Nd(NO_3)_3$. CeCl_ acts as a cathodic inhibitor, while other salts act as mixed cathodic/anodic inhibitors. An important result



Figure 3: Electronic structure of benzimidazole molecule interacting with Cu(111) surface: charge density difference (top) and molecule and Cu projected density of states (bottom).

was that a mixture of salt has a synergetic effect. Conversion coatings were prepared at different times of immersion and different temperatures. At room temperature the most effective protection was achieved by $Ce(NO_3)_3$ coatings. At higher temperature, 60 °C, conversion coatings based on $La(NO_3)_3$ and $Ce(NO_3)_3$ exhibited better protection. The mechanism of inhibitions was dependent on the type of inhibitor. The $Ce(NO_3)_3$ coating is formed at the whole surface, while $La(NO_3)_3$ and $Nd(NO_3)_3$ coatings are formed at the intermetallic sites of copper and zinc.

Investigations of natural compounds as potentials inhibitors of the corrosion of metals open new possibilities for the elimination of toxic and hazardous organic inhibitors. Among these socalled green inhibitors we have investigated phytic acid or inositol hexakisphosphate (IP₄). It is found in natural plants, especially seeds and bran. Self-assembled monolayers are liable to form dense and stable films on the surface, which can protect the metal against the corrosion process. The corrosion resistance in a 3% NaCl solution was studied by electrochemical measurements as a function of the preparation method, including surface roughening, time of immersion and inhibitor concentration. The results indicate that the most effective pretreatment was the oxidationreduction cycle in 2-M H₂SO, which increased the roughness of the copper surface and its contact angles. The best corrosion effectiveness was achieved at a concentration of phytic acid of 0.1 mM and an optimum immersion time of 6 hours. Self-assembled layers of phytic acid can be used as a cheap, non-toxic inhibitor against the corrosion of copper in chloride solution reaching inhibitor effectiveness around 80 % under optimal conditions. X-ray photoelectron analysis proved that IP chemically bonds to the metal surface. Within the search of environmental friendly inhibitors the carboxylic acids were also tested for the corrosion of copper, zinc and brasses in artificial rain. The carboxylic acids form by self-assembling a hydrophobic layer on the surface which improves the corrosion resistance of underlying metals. The surface of metals was modified by immersing the samples in ethanol solution of different carboxylic acids: hexanoic, decanoic, myristic and stearic. The corrosion resistance increases with the length of the aliphatic tail of carboxylic acid.

We investigated the influence of surface roughness on the formation of hydrophobic layer and corrosion resistance. For a given carboxylic acid, samples with higher surface roughness have better corrosion resistance. The process of self-assembling is fast, as corrosion protection was achieved after only one minute of immersion in an inhibitor solution. Myristic and stearic acids exhibited over 95 % inhibition effectiveness on copper and brass. For zinc these acids were less effective (about 60 %).

Experimental electrochemical methods combined with quantum chemical calculations and molecular dynamics simulations were used to investigate the possibility of exploring various amino acids as "green" corrosion inhibitors for copper in hydrochloric acid. Among eleven amino acids studied, cysteine achieved the highest inhibitor effectiveness reaching 52% at 10-mM concentration. Other amino acids reached an effectiveness less than 25%, some of them even acted as corrosion accelerators. Based on the experimental results, theoretical calculations and simulations were focused on cysteine and alanine. The electronic and reactivity parameters of their protonated forms in an electrical double layer were evaluated by density

 $CH_2CIOONO_{tp} + NO_2$

Figure 4: NO2-assisted nitrite-nitrate isomerisation transition state.

functional calculations. In addition, molecular dynamic simulations were introduced to follow the adsorption behaviour of these two amino acids at the Cu(111) surface in the electrolyte solution. The results indicate that the orientation of both molecules is nearly parallel to the surface, except that of the ammonium group, which is directed away from the surface. Therefore, as the orientation of the cysteine and alanine molecules at the surface is similar, the thiol functional group is responsible for the superior inhibition efficiency of cysteine.

We continued with the study of organic corrosion inhibitors (i.e., molecules that have the ability to inhibit the corrosion). Our principal aim is to better understand how organic corrosion inhibitors act against corrosion at the

molecular level and to discern the fundamental principles that govern their corrosion inhibition characteristics. In the past few years we have studied by means of first-principle density-functional-theory (DFT) based computer simulations the interaction of several azole type corrosion inhibitors with surfaces of copper, iron, and aluminium. Our findings indicate that the inhibitor-surface bonding strongly depends on the type of metal. Due to obvious modelling reasons the majority of DFT calculations were performed at the solid/vacuum interface. Nevertheless, we have recently extended these

calculations and also considered the solid/liquid interface, because corrosion takes place at this phase boundary. In this context, we examined the interaction of imidazole, triazole, and tetrazole inhibitors with surfaces of copper. Molecules in protonated, neutral, and deprotonated forms were considered so as to ascertain how the molecule-surface interaction depends on the »acid-base« molecular form. We have shown that chemisorptive bonding is the strongest for deprotonated inhibitors. This preference is particularly strong for triazole and tetrazole, while for imidazole the aqueous-phase adsorption free energy of the neutral form is comparable to that of deprotonated form. This suggests that for imidazole – because of its more basic nature – the neutral form and for triazole and tetrazole and tetrazole their deprotonated forms are the active species for inhibiting corrosion.

With respect to a long-term goal of developing more predictive models for screening new corrosion inhibitors with potentially superior corrosion inhibition characteristics, we were able – on the basis of the ascertained atomic scale details of the inhibitor-surface interactions – to pinpoint some inconsistencies in the usual application of a few electronic parameters that are frequently used in this context and are based on the so-called HSAB (*hard and soft acids and bases*) concept. Theoretical formalization of the HSAB concept has been derived for molecular systems, yet in the context of corrosion inhibitors one deals with surfaces that are extended systems. This leads to some ambiguities, which are the source of the above-mentioned inconsistencies. We have shown how these HSAB-based electronic parameters can be consistently applied in the case molecular-surface systems.

Our theoretical investigations of atmospherically relevant radical reactions were based on quantum chemical methods and in this year were focused on the examination of the mechanism of the singlet radical-radical reaction of the CH_2ClO_2 with NO. The chlorine-containing peroxy radical CH_2ClO_2 appears in the atmosphere as an intermediate in the oxidation of methyl chloride originating from oceans, volcano eruptions and vegetation burning. In general, the mechanism can be summarized as the initial association of radicals, followed by isomerization and/or the dissociation of intermediates. The association by forming the N-O bond is an energetically

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

By means of first-principle density-functional-



Figure 5: Green, efficient and selective aerobic oxidation of alcohols.

favorable process occurring without barrier. The $CH_2CIOONO$ intermediate possesses two conformational forms, the very low rotational barrier makes their interconversion likely. While the only pathway for the cis-perp $CH_2CIOONO$ is homolytic dissociation to form the $CH_2CIO + NO_2$ products, the trans-perp $CH_2CIOONO$ is also open for the rearrangement to nitrate. The barrier for rearrangement that must be surmounted is very high, but it has been shown that one NO_2 molecule stabilizes the transition state for nitrite-nitrate transformation. NO_2 -assisted isomerization reduces the activation energy significantly, being below the free reactants energy level, implying that the nitrite-nitrate isomerization process would be possible. The subsequent decomposition of CH_2CIONO_2 results in three reaction channels. The lower energy channel is the elimination of nitrous acid with the simultaneous production of CHCIO, while the elimination of formaldehyde accompanying with the formation of either c-CIONO or $CINO_2$ products is somewhat less favorable.

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

We have demonstrated that the nitrite-nitrate isomerization in the CH_2CIO_2 radical reaction with NO is significantly facilitated by the assistance of a single NO₂ molecule compared to the unimolecular isomerization.

a green, efficient and selective method for the oxidation of alcohols to corresponding carbonyl derivatives using air oxygen under the catalytic support of a three-component system: *ammonium nitrate / nitroxyl radical / strong acid*. The method was verified on the broad selection of different structural types of alcohols, including those bearing heteroatoms. The scale-up experiment was performed, revealing the potential convenience also for industrial application. On the basis of this knowledge we invented and

developed a new method for the aerobic chlorination of organic compounds using the reaction system: air / am-monium nitrate(cat) / moleculare iodine(cat) / 36% aqueous HCl and established its efficiency and selectivity in the case of the transformation of methyl ketone derivatives in their chloromethyl analogues. Each component of the reaction system was found to be essential for its efficiency. We proved that the first step of the reaction is aerobic iodination, catalysed by the redox cycle of nitrogen oxides, followed by a halogen-exchange process and the oxidative regeneration of released iodide so continuing the process. We further investigated the use of polyvalent iodine compounds as iodinating reagents and invented a new method for the catalytically supported oxidation of the iodination of organic compounds, thus overcoming the low reactivity of molecular iodine and increasing the green profile of the iodination process.

We investigated the transformations of alcohols with N-halosuccinimides in aqueous media or under solvent-free reaction conditions. Tertiary benzyl alcohols could be directly transformed to vicinal halohydrines in aqueous media

We have developed a green, efficient and selective method for the oxidation of alcohols to the corresponding carbonyl derivatives using air oxygen under the catalytic support of a threecomponent system: *ammonium nitrate / nitroxyl* radical/ strong acid. or in vicinal halo-methoxy derivatives in methanol solvent. We discovered that N-halo compounds could be efficient catalysts for transformations of primary, secondary and tertiary benzyl alcohols into the corresponding derivatives, where the hydroxyl group is directly substituted with a different nucleophile.

In the framework of the syntheses of organic peroxides as potential bioactive compounds we were continuing the investigation of an efficient transformation of different substrates to structurally varied model organic peroxides and tested antibacterial bioactivity.

In the framework of the Centre of Excellence CIPKeBiP and the collaboration of the high-tech company ACIES BIO we were continuing investigations of the directed synthesis of potential bioactive compounds from the family of pantothenic acid and derivatives of maleic acid as precursors in polyketide biosynthesis. We have continued the collaboration with the company Semenarna on the synthesis of gamethocydic active compounds used in the processes of the production of plant hybrids and with the company ECOT in the development of new products used in non-human cosmetics. At the Jožef Stefan International Postgraduate School we teach two organic greenchemistry courses.

Some outstanding publications in the past year

- Milošev, I., Žerjav, G., Calderon Moreno, J. M., Popa, M.: Electrochemical properties, chemical composition and thickness of passive film formed on novel Ti-20Nb-10Zr-5Ta alloy, Electrochim. Acta, 99 (2013), 176–189
- Milošev, I., Blejan, D., Varvara, S., Muresan, L. M.: Effect of anodic oxidation on the corrosion behaviour of Ti-based materials in simulated physiological solution, J. Appl. Electrochem., 43 (2013), 645–658
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- 4. Lesar, A.: Mechanistic study on the reaction of the CH₂ClO₂ radical with NO, Chem. Phys. Lett., 579 (2013), 28-34

- R. Prebil, Laali, K. K., S. Stavber, Metal and H₂O₂ free aerobic oxidative aromatic halogenation with [RNH₃⁺] [NO₃⁻]/HX and [BMIM(SO₃H)][NO₃)_x(X)_y] (X = Br, Cl) as multifunctional ionic liquids. Org. Lett., 15 (2013), 2108–2111
- 6. Bedrač, L., Iskra, J.: Iodine(I) reagents in hydrochloric acid-catalyzed oxidative iodination of aromatic compounds by hydrogen peroxide and iodine, Advanced Synthesis & Catalysis, 355 (2013), 1243–1248

Awards and appointments

- 1. Leon Bedrač: Krka Awards for PhD Thesis, Novo mesto, Slovenia, 2013
- 2. Sebastjan Peljhan: Maks Samec Awards for PhD Thesis in the field of Chemistry, Ljubljana, Slovenia, 2013
- 3. Peter Rodič, Ingrid Milošev, Jernej Iskra, Barbara Kapun: 1st prize at the 6th International Conference for technology transfer together with Innovation Day of the Chamber of Commerce of Slovenia for innovation with largest market potential after the selection of local and foreign experts in the field of technology transfer and representatives of domestic and foreign venture capital, 2013

Organization of conferences, congresses and meetings

1. Fourth Regional Symposium on Electrochemistry, South-East Europe - RSE-SEE, Ljubljana, Slovenia, 26. 5. – 30. 5. 2013

Patent granted

1. Primož Titan, Jernej Iskra, Vladimir Meglič, Chemical hybridization of hermaphrodite plant species with easily soluble derivatives of oxanilic acid, SI24033 (A), Urad RS za intelektualno lastnino, 30.10.2013.

INTERNATIONAL PROJECTS

- CARISMA; Catalytic Routines for Small Molecule Activation COST Office Asst. Prof. Jernej Iskra
- Asst. Froi. Jernej Iskra
 Transformations of Organic Compounds under Green Reaction Conditions Slovenian Research Agency
- Prof. Stojan Stavber
 Improvement of Functionality of Biomedical and Engineering Materials Slovenian Research Agency
 Prof. Ingrid Milošev

RESEARCH PROGRAMS

- 1. Multiphase Nanoarchitectures: Development, Physical-Chemical Characterization and Simulation of Processes
- Prof. Ingrid Milošev 2. Bioanorganic and Bioorganic Chemistry Prof. Stojan Stavber

R&D GRANTS AND CONTRACTS

 Modifications of Surface of Metallic Biomaterials and Their Interaction with Bio-Environment Prof. Ingrid Milošev

VISITORS FROM ABROAD

- 1. Selma Özarslan, Ph. D. Student, Mustafa Kemal University, Science and Art Faculty, Department of Physics, Antaky - Hatay, Turkey, 18. 3.-23. 9. 2013
- Prof. Osman Sahin, Mustafa Kemal University, Science and Art Faculty, Department of Physics, Antaky - Hatay, Turkey, 5. 6. 2013

- Use of Green Energy Sources: New Functional Nanomaterials on the Base of Polyoxometalates and TiO2 Nanostrucutres for Production of Hydrogen by Catalytic Oxidation of Water – NANOleaf Asst. Prof. Jernei Iskra
- New Technology for Design of Novel Polyketide Drug-Leads with Chemically Ameanable Moieties Prof. Stoian Stayber
- SURFUNCTI: Controlled Surface Structuring and Surface Functionalisation of Advanced Biomedical Titanium Alloys for Ortopaedic Implants Prof. Ingrid Milošev

NEW CONTRACTS

- 1. Development of New Synthetic Protocols Acies Bio, d. o. o. Prof. Stojan Stavber
- New Technology for Design of Novel Polyketide Drug-Leads with Chemically Amenable Moieties
 - Acies Bio, d. o. o. Prof. Stojan Stavber

 Prof. Silvia Cere, INTEMA, Division of Electrochemistry and Corrosion, Universidada Nacional de Mar del Plata, Argentina, 24. 6.–6. 7. 2013



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- 1. Asst. Prof. Jernej Iskra
- 2. Dr. Anton Kokalj
- Dr. Antonija Lesar
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- Prof. Ingrid Milosev, Head
 Prof. Stojan Stavber
- Postgraduates
- 6. Dr. Leon Bedrač, left 01.09.13
- 7. Dr. Nataša Kovačević, left 01.07.13
- 8. Jerca Pahor, B. Sc.
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ORIGINAL ARTICLE

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- 9. Antonija Lesar, "Mechanistic study on the reaction of the $\rm CH_2ClO_2$ radical with NO", Chem. Phys. Lett., vol. 579, pp. 28-34, 2013.
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- 11. Ingrid Milošev, Julija Hmeljak, Andrej Cör, "Hyaluronic acid stimulates the formation of calcium phosphate on CoCrMo alloy in simulated physiological solution", *J. mater. sci., Mater. med.*, vol. 24, no. 3, pp. 555-571, 2013.
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9. Dunia Peca, B. Sc.

10. Rok Prebil, B. Sc.

11. Peter Rodič, B. Sc.

12. Katarina Starkl, B. Sc.

Barbara Volarič, B. Sc.
 Dr. Dejan Vražič, left 01.04.13

13. Simona Tušar, B. Sc.

16. Gregor Žerjav, B. Sc.

17. Barbara Kapun, B. Sc

Technical officer

1. Katarina Starkl, Janez Mravljak, "Zdravljenje in preprečevanje malarije", *Farm. vestn.*, vol. 64, no. 5, pp. 371-379, dec. 2013.

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- Andrej Cör, Julija Hmeljak, Mitja Rak, Maja Čemažar, Ingrid Milošev, "Pathophysiological mechanisms of joint impant loosening", In: *The Partners and the Objectives of the Trans2Care, and Italy-Slovenia cross border network of science and healthcare institutions*, Sabina Passamonti, ed., Trieste, Edizioni Università di Trieste, 2013, pp. 99-102.
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Mentoring

- 1. Leon Bedrač, *lodine(l) compounds: catalysts for iodination of organic molecules:* doctoral dissertation, Ljubljana, 2013 (mentor Jernej Iskra).
- 2. Nataša Kovačević, *Interactions of azole corrosion inhibitors with transition metal surfaces:* doctoral dissertation, Ljubljana, 2013 (mentor Anton Kokalj; co-mentor Ksenija Kogej).
- 3. Dejan Vražič, *The Role of Iodine and N-Halo Compounds in Transformations of Organic Molecules:* doctoral dissertation, Ljubljana, 2013 (mentor Marjan Jereb; co-mentor Stojan Stavber).

ELECTRONIC CERAMICS DEPARTMENT

K-5

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

In the framework of lead-free piezoelectric materials we were particularly interested in alkali-niobate-based ceramics, which are still considered as one of the most important candidates for the replacement of lead-based perovskites in piezoelectric applications. In collaboration with Keio University from Japan we developed a new synthesis method for the preparation of fine and single-phase potassium sodium niobate (K_{0.5}Na_{0.5}NbO₃) powders. The method consists of the attrition milling of fine Nb₂O₅ particles suspended in an ethanol solution of sodium and potassium acetates. We obtained a single-phase KNN powder by calcining the milled powder twice at Head: temperatures as low as 450-650°C, which are 100-200°C lower than those typically used during the conventional Prof. Barbara Malič solid-state synthesis of KNN.

Using optical dilatometry and a detailed microstructural analysis we studied the sintering behaviour of sodium niobate (NaNbO3) powders with particles of nanometre and submicrometre sizes. We found that the initial particle size did not affect the evolution of the microstructure upon annealing, suggesting a key role of the mechanisms responsible for the grain growth in the initial stage of the sintering. By measuring the specific surface area of the specimens, which were annealed at different temperatures, we found that the observed grain growth is due to the surface diffusion. Owing to the low activation energy (50-60 kJ/mol), in fact,

this grain-growth mechanism is activated in the initial stage of the sintering and, thus, decreases the driving force for the sintering and prevents any further densification of the powder compact. NaNbO, ceramics with a relative density of 98% and an average grain size of $0.7\pm0.29 \,\mu\text{m}$ were successfully prepared by hot pressing at 1150°C. The results significantly contribute to the general understanding of the sintering of alkali-niobate-based ceramics and suggest ways to control the microstructure of this important group of lead-free piezoceramics.

Within the activities on lead-based piezoelectric ceramics, we focused on the solid-state synthesis and characterization of the Pb(Zr,Ti)O, (PZT) ceramics, mechanically toughened by tetragonal-stabilized zirconia (TZ) particles. In order to achieve a homogeneous distribution of TZ grains within the PZT matrix, we developed a modified solid-state synthesis procedure, consisting of pre-milling, pH adjustment and a modification of the surface of the TZ powder. According to the Voronoi-diagram analysis of the microstructures of the ceramics, the modified synthesis route provided a more homogeneous TZ distribution in the PZT matrix, as compared to the composites processed by conventional means (figure 1). The R-curve measurements, performed at the Technische Universität Darmstadt, however, did not show a measureable difference in the fracture behaviour of the two PZT-TZ composites.

Within the 7FP EU project CERAMPOL and in collaboration with the company HIPOT-RR we continued our work on the integration of piezoelectric PZT actuators in waste-water cleaning systems. Based on the vibration measurements of a corundum substrate with integrated piezoelectric actuators, we were able to evaluate the influence of various parameters, such as the type of the piezoelectric material and the position of the actuators, on the amplitude and frequency of the substrate vibration resonances. A numerical analysis of the different substrate/actuator structures showed trends in the vibration behaviour. A combination of the numerical analysis and the experimental verification made it possible to identify the main parameters of the vibration system, like those mentioned above, which will be further optimized within the project.

As a co-author, Tadej Rojac published a review article on mechanochemical synthesis entitled "Hallmarks of mechanochemistry: from nanoparticles to technology" in the high-impact journal Chemical Society reviews, 2013, 42, 7571 (impact factor for 2012: 24.89).



Figure 1: The area size distribution of the Voronoi polygons of PZT-TZ composites prepared by modified (a) and non-modified (b) synthesis methods. The insets show the Voronoi diagrams.

a) (012) (101) (a.u.) (900) (110) (018) (104) (0010) (0012) (600) (003) (107) m 30 60 20 20⁴⁰(°) 50 10 µm

Figure 2: X-ray diffraction pattern (a) and microstructure (b) of $CuAlO_2$ ceramics, sintered at 1100°C for 2 hours in air. The inset shows a photo of the ceramic sample.

The 0.57Pb(Sc1/2Nb1/2)O3-0.43PbTiO3 (PSN-PT) is a perovskite material that can be used in various piezoelectric applications, including sensors, actuators and ultrasound transducers. The integration of such functional materials onto substrates in the form of thin or thick films often results in thermal stresses in the film, which have their origin in the mismatch between the thermal expansion coefficient of the active layer and the substrate, and may significantly affect the functional response of the material. In order to understand and control these stresses, the linear expansion coefficient of the PSN-PT must be known, in both the unpoled and poled states. We found that the thermal expansion coefficient of PSN-PT increases from 30°C up to the Curie temperature of 260 °C, where it reaches $2.08 \cdot 10^{-6}$ K⁻¹. The phase transition was identified as an anomaly in the expansion between 260 °C and 280 °C. The coefficient of thermal expansion then increases with a further increase in the temperature, reaching 9.66 · 10⁻⁶ K⁻¹ at 400 °C. These data will be essential for the integration of PSN-PT in thin- or thick-film structures.

In collaboration with the Ecole Polytechnique Fédérale de Lausanne, Switzerland, we studied the **elastic properties of Pb(Mg_{1/3}Nb_{2/3})O₃ (PMN) ceramics**. It was shown that the PMN ceramics exhibit true anelastic relaxor behavior with the parameters of the Vogel-Fulcher equation similar to those for dielectric relaxation.

We continued our research on **multiferroic BiFeO**₃ ceramics, focusing on the (Bi,RE)FeO₃ (RE=Sm, Gd, Dy) compositions, which exhibit morphotropic phase boundaries. By combining the milling of the starting powders in ethanol with the addition of polyacrilic acid and subsequent mechanochemical activation, we succeeded in preparing homogeneous powders with the sintering temperatures as low as 800°C. The powders were then used to prepare homogeneous and dense bulk ceramics. Like in the case of BiFeO₃, the ceramics modified by the RE oxides exhibited large electric-field induced strains, which exceeded 0.3%. The advantage of these modified ceramics over the unmodified BiFeO₃ is that the strain shows little dependence on the driving electric-field frequency; as compared to unmodified BiFeO₃, the response of RE-modified ceramics is thus more stable.

In collaboration with the Department for Condensed Matter Physics we studied the electrocaloric (EC) response of $0.7Pb(Mg_{1/3}Nb_{2/3})O_3-0.3PbTiO_3$ bulk ceramics, processed from mechanochemically activated powders. The highest temperature change of 2.7 K was observed in the vicinity of the critical point, i.e., at 430 K, and under an applied electric field of 90 kV/cm. In addition, we investigated the EC response of the environmentally friendly lead-free relaxor $K_{0.5}Na_{0.5}NbO_3$ -STTIO₃ (KNN-STO) ceramics. The results confirmed the large EC response in the vicinity of the dielectric anomaly. The EC temperature change at room temperature is comparable to that measured in lead-based ceramics.

Using the inkjet printing of water-based dispersions of submicron lead zirconate titanate (PZT) particles we prepared films with thicknesses of a few micrometres. We confirmed the local piezoelectric response of such PZT films by means of piezo-response force microscopy. In the framework of **lead-free ferroelectric thin films** prepared by Chemical Solution Deposition, we collaborated with the Ecole Centrale Paris, France, and investigated the phase transitions of KNN thin films deposited onto (111)Pt/TiO₂/SiO₂/Si substrates. The purpose was to compare the phasetransition behaviour of the KNN films with two different microstructures, i.e., columnar and granular. Raman spectroscopy and X-ray diffraction analysis confirmed the presence of both phase transitions as observed in the KNN powder, i.e., the monoclinic-to-tetragonal (T_{m-T}) and the tetragonal-to-cubic (T_{T-C}). Whereas the T_{m-T} transition of the film with the columnar microstruc-

ture was similar to that observed in the KNN powder, the Curie temperature (T_{T-c}) was slightly lower. We attribute this lowering of the T_c to the presence of tensile stresses, which develop as a consequence of the thermal expansion coefficient mismatch between the film and the substrate.

Within the project FERROPATCH in the frame of the program JP PECS of the European Space Agency (ESA) we prepared Ba_{0.5}Sr_{0.5}TiO₃ (BST) thin-film varactors on alumina substrates. Single-phase and dense films with homogenous microstructures and thicknesses between 70 nm and 600 nm were prepared by annealing the asdeposited films at temperatures up to 900°C. The highest dielectric permittivity was measured in the 170-nm-thick sample and was 1310 at 100 kHz and 1210 at 10 GHz. In addition, we also studied the synthesis of BST nanoparticles,

which were prepared via the thermal degradation of acetylacetone precursors in oleylamine under the presence of stearic acid, used as surfactant. The particles were amorphous and crystallized into the perovskite phase after annealing at 700 $^{\circ}$ C.

The work within the 7FP EU ORAMA project was concentrated on the synthesis of oxide semiconductors and dielectrics for **transparent electronics**. $CuAlO_2$, which is a p-type semiconductor, was synthesized by annealing a stoichiometric mixture of nano-boehmite (AlOOH) and Cu_2O at 1100°C in an argon atmosphere. In contrast to the conventional synthesis from a mixture of oxide powders, this synthesis method represents an efficient way toward the phase-pure delafossite. By sintering the as-prepared powder compacts at 1100°C for 2 hours in air, we succeeded in preparing X-ray-diffraction phase-pure ceramics with 86% of relative density, which can be used as sputtering targets (figure 2).

Our studies related to thin dielectric films with a high permittivity for transparent electronic components were focused on thin films based on Ta_2O_5 and Ta_2O_5 -Al $_2O_5$ -SiO $_2$, which were prepared by Chemical Solution Deposition. The films, deposited onto glass substrates and processed at temperatures up to 400°C, showed an optical transmittance of ~80 %, a dielectric permittivity of ~20 and a low leakage current. These films are thus suitable for use in thin-film capacitors or transistors. In addition, we adopted inkjet printing for the deposition of thin films of n-type conducting oxides based on ZnO and SnO₂ onto various substrates.



Figure 3: PZT thick film on the Pt/Al2O3 substrate prepared by inkjet printing. a) scanning electron microscopy (SEM) image of the crosssection b) atomic-force miscoscopy (AFM) image and c) out-of-plane amplitude PFM image of the surface of the PZT thick film; d) local d33(V) hysteresis loop obtained from a selected area on the film.

Within the research on the processing of **piezoelectric thick films** by the **electrophoretic deposition (EPD) process**, we systematically studied the influence of the polyacrylic acid / organic base ratio on the electrical conductivity of the dispersion and on the thickness uniformity of the as-deposited layers. At the optimal polyacrylic acid / organic base ratio we obtained a stable dispersion of donor-doped PZT particles in ethanol with a low electrical conductivity. The deposited layer had a thickness of $30\,\mu$ m and was uniform and homogeneous. The dispersions were used for the processing of thick films on curved porous PZT substrates. In the next step and in collaboration with

researchers from François-Rabelais University from Tours, France, we fabricated geometrically-focused high-frequency ultrasound transducers (US) for medical diagnoses. With the colleagues from Tours we also investigated the functional properties of $0.65Pb(Mg_{1/3}Nb_{2/3})O_3-0.35PbTiO_3$ (PMN-PT) thick films for US transducers. The results suggest that the PMN-PT thickfilms transducers are superior to those made from the standard Pb(Zr,Ti) O, (PZT) piezoelectric material.

We fabricated a ceramic micro reactor with large cavities for the catalytical production of hydrogen from methanol and water by using LTCC technology.

We studied the preparation of PZT ceramics with a controlled amount, size and distribution of pores, which could be used as substrates for high-frequency ultrasound transducers. The method consists of the heterocoagulation of PZT and polymethyl methacrylate (PMMA) particles.

We developed a procedure for the processing of aqueous dispersions of ceramic particles, suitable for the patterning of thick films by piezoelectric inkjet printing. We reduced the average particle size of a micron-sized PZT powder to a few tens of nanometres by milling and provided an effective dispersion of PZT particles in water by controlling the pH of the dispersion, and the type and amount of dispersant. The ink with an optimized average PZT particle size, surface tension and viscosity was inkjet printed onto platinised corundum substrates. The inkjet printed structures, dried and fired at 1100°C, were dense and \sim 5 µm thick. The local piezoelectric response of the PZT film was confirmed using ab atomic force microscope equipped with a piezoresponse-force module (figure 3).

By optimizing the rheological properties of the ink we improved the procedure for the processing of KNN thick films using screen-printing technology. The films were deposited onto substrates with different thermal expansion coefficients, so that different degrees of in-plane biaxial stresses were induced in the films. The influence of these stresses was reflected in the structural and functional properties of the films. The most important is the phenomenon of 'self-poling' of the KNN thick films, the extent of which depended on the mechanical stresses, i.e., on the type of the substrate.

We continued the investigations on LTCC (Low Temperature Co-fired Ceramics), used for the fabrication of 3D structures for different electromechanical (MEMS - Micro Electro Mechanical Systems) and chemical microsystems. In collaboration with the partners from Montanuniversität Leoben, Austria, we studied the influence of the firing conditions on the microstructure and mechanical properties of Du Pont LTCC. We concluded that the porosity has a major influence on the elastic modulus, the fracture toughness, the hardness and the biaxial flexural strength



Figure 4: LTCC reactor for high-temperature catalytic production of hydrogen from methanol and water. The external dimensions of the structure are 90 mm \times 90 mm \times 9.2 mm and the volume of the buried cavities is 18.7 cm³. The figure shows the bottom part of the reactor with nine supports.

of the LTCC. If the LTCC materials are fired at elevated temperatures for prolonged periods, so that the porosity is reduced, their properties remained unchanged, regardless of the firing temperature and/or firing time. This finding is important for the design and production of ceramic pressure sensors and other MEMS devices, which require relatively long firing procedures at higher temperatures, as compared to the conditions usually required for the processing of LTCC. In 2013 we reinforced the collaboration with KEKO Oprema d.o.o. in the field of materials and technologies based on LTCC.

Traditional co-operation with the research partners from HIPOT-RR and Centre of Excellence NAMASTE continued in all the research projects related to thick-film and LTCC technology. With the group from the company KEKON d.o.o. we continued our research in the field of functional thick-film materials, in particular, we investigated **new thick-film lead-free resistors** as possible sensor elements. We found that the temperature dependence of resistivity of these materials satisfies the needs for the application, however, the "gauge" factors, i.e., the dependence of the resistivity on the deformation, are three times lower than required, so that these materials are not suitable as pressure sensors. We also tested a commercial ESL 3411-1 thick-film resistor with a **high and linear dependence of resistivity versus temperature** and a low sheet resistivity. The results suggested that this material is compatible with LTCC tapes and that it could be used for temperature measurements over large surfaces. This material was successfully used as a sensor for temperature control and regulation in large LTCC chemical reactors.

Within the programme JE PECS of the European Space Agency (ESA), we continued our work on the CERACON project, together with the partners from the Department of Systems and Control, and the National Institute of Chemistry. The topic of the project was the **design and fabrication of LTCCbased micro reactors** and the necessary periphery for the high-temperature

catalytic transformation of methanol and water into hydrogen. It is worth mentioning that we succeeded in designing and constructing two reactors, i.e., one for the steam reforming and the other for the removal of the residual carbon monoxide from gas products. Both reactors had large buried cavities where the chemical reactions take place; the volume of the reformer and the reactor for CO removal was 18.7 cm³ and 5.4 cm³, respectively. These, rather extreme dimensions for LTCC technology, were fabricated in order to satisfy the required production of 85 litres of hydrogen per hour. The realisation of these **particularly large cavities** required special LTCC lamination procedures and a controlled firing process. The final dimensions of the reformer and the reactor for CO-removal were, respectively, 90 mm × 90 mm × 9.2 mm and 90 mm × 36 mm × 9.2 mm (figure 4).

In collaboration with the company ETI d.d. Izlake we investigated various silicate materials, i.e., steatite and cordierite, which are used in electrical engineering as heat or electrical insulators. We systematically studied the influence of raw materials on the microstructure, mechanical and electrical properties of the ceramics. At the optimal amount of selected raw materials and at the optimal milling conditions we prepared a new type of dense, alkaline steatite with a high flexural strength (~185 MPa) and a high specific electrical resistivity (~0.8 M Ω m). The resulting material was prepared on a production scale in the company and is now used for the fabrication of electrical fuses.

Some outstanding publications in the past year

- Baláž, P., Rojac, T., et al.: Hallmarks of mechanochemistry: from nanoparticles to technology. Chemical Society reviews, vol. 42, 7571–7637, 2013, doi: 10.1039/C3CS35468G [COBISS.SI-ID 26654759]
- Hreščak, J., Benčan, A., Rojac, T., Malič, B: The influence of different niobium pentoxide precursors on the solid-statesynthesis of potassium sodium niobate, J. Eur. Ceram. Soc., vol. 33, 3065–3075, 2013, doi: 10.1016/j. jeurceramsoc.2013.07.006
- Vojisavljević, K., Malič, B., Mamoru, S., Drnovšek, S., Kosec, M.: Solid state synthesis of nano-boehmite-derived CuAlO2 powder and processing of the ceramics, J. Eur. Ceram. Soc., vol. 33, 3231–3241, 2013, doi: 10.1016/j. jeurceramsoc.2013.05.025
- Kuščer, D., Noshchenko, O., Uršič, H., Malič, B.: Piezoelectric properties of ink-jet printed lead zirconate titanate thick films confirmed by piezoresponse force microscopy, J. Am. Ceram. Soc., vol. 96, 2714–2717, 2013, doi: 10.1111/jace.12532

 Kupec, A., Gemeiner, P., Dkhil, B., Malič, B.: Phase transitional behavior of potassium sodium niobate thin films, Thin solid films, vol. 539, 317–322, 2013, doi: 10.1016/j.tsf.2013.05.098

Organization of conferences, congresses and meetings

1. COST Training school on characterization of materials, Ljubljana, Slovenia, 28.-29. 1. 2013

Patent granted

- Luca Gregoratti, Marco Peloi, Marija Kosec, Danjela Kuščer, Giuseppina Palma, A material in the form of lithium fluoride powder containing colour centres, method for preparation and use thereof, US8535434 (B2), US Patent Office, 17.9.2013.
- 2. Kostja Makarovič, Janez Holc, Darko Belavič, Marko Hrovat, Marija Kosec, Multilayer ceramic structures for non-contact dielectric heating of liquids, SI24008 (A), Urad RS za intelektualno lastnino, 30.8.2013.
- 3. Marina Santo-Zarnik, Darko Belavič, Marjan Hodnik, Sandi Kocjan, A pressure-sensor module with a ceramic cantilever sensing structure, SI24085 (A), Urad RS za intelektualno lastnino, 29.11.2013.

INTERNATIONAL PROJECTS

- 7FP ORAMA; Oxide Materials Towards a Matured Post-silicon Electronics Era European Commission Prof. Barbara Malič
- 7FP CERAMPOL; Ceramic and Polymeric Membrane for Water Purification of Heavy Metal and Hazardous Organic Compound European Commission
 - Asst. Prof. Danjela Kuščer Hrovatin
- 7FP PI; The Piezo Institute European Expertise Centre for Multifunctiona and Integrated Piezoelectric Devices European Commission
- Prof. Barbara Malič
- 4. CERACON; Integration and Control of Liquid Fuel processor based on Ceramic Micro-Systems
- ESA/ESTEC Asst. Prof. Marko Hrovat
- COST MP0904; SIMUFER: Single- and Multiphase Ferroics and Multiferroics with Restricted Geometries COST Office
- Prof. Barbara Malič
- FERRO-PATCH; Frequency and Polarisation Agile Microstrip Patch Antenna based on Ferrelectric Varactors ESA/ESTEC
- Prof. Barbara Malič
- Solution Processing of Thin Films for Transparent Electronics (TRANS) Slovenian Research Agency Prof. Barbara Malič
- Baloara Malic
 Dielectric Spectroscopy and Tunability of Low-Temperature Rocessed Complex Perovskites
 - Slovenian Research Agency Prof. Barbara Malič

RESEARCH PROGRAM

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

VISITORS FROM ABROAD

- 1. Julian Walker, School of Materials Science & Engineering, University of New South Wales, Sydney, Australia, 1. 1.–31. 7. 2013
- 2. Prof. Liliana Mitoseriu, University "Al. I. Cuza", Faculty of Physics, Iasi, Romania, 23.– 30. 1. 2013
- Dr. Denis Schütz, CD-Lab for Advanced Ferroic Materials, Graz, Austria, 27. 1.–14. 4. 2013
 Dr. Madaida Horshidan, University "ALL Cuza", Faculty of Physics, Iasi, Pompania, 27.
- Dr. Nadejda Horchidan, University "Al. I. Cuza", Faculty of Physics, Iasi, Romania, 27. 1.-22. 2, 2013
- 5. Andre-Pierre Abellard, Université François Rabelais, Tours, France, 2.-29. 3. 2013

R&D GRANTS AND CONTRACTS

- 1. Nanostructures for High-Efficiency Solar Cells and Photovoltaic Prof. Barbara Malič
- Oxide-Based Components for Transparent Electronics Prof. Barbara Malič
- Tunable Ferroelectric Thin Film Capacitors for Agile Microwave Antennas Prof. Barbara Malič
- High-performance Piezoelectric Materials for Sensors and Actuators in Hightemperature Applications
- Asst. Prof. Tadej Rojac 5. Textured Ceramic Films for Sensors and Actuators
- Asst. Prof. Tadej Rojac
- 6. Materials and Technologies for Chemical Microsystems Asst. Prof. Andreja Benčan Golob
- Pb(Sc0.5Nb0.5)03-PbTiO3 Thick Films for Sensor and Actuator Applications Dr. Hana Uršič Nemevšek

NEW CONTRACTS

- Evolution of Microstructure in Non-porous Bulk Ceramics with Selected Properties for Applications in Low Temperature Cofired Ceramic (LTCC) structures Kekko – Oprema, d. o. o., Žužemberk
- Prof. Barbara Malič
 Materials and Technologies for Chemical Microsystems Keko – Oprema, d. o. o., Žužemberk Asst. Prof. Andreja Benčan Golob
- Nanomaterials in Ceramics-Feasibility Study RC eNeM Prof. Barbara Malič

- Pierrick Chevreux, Ecole Nationale Supérieure Céramique Industrielle, Limoges, France, 3. 3.-7. 6. 2013
- Prof. Dragan Damjanovic, Swiss Federal Institute of Technology-EPFL, Lausanne, Switzerland, 6.–9. 3. 2013
- Dr. Marco Deluca, Institut f
 ür Struktur- und Funktionskeramik, Montanuniversit
 ät Leoben, Materials Center Leoben Forschung GmbH, Leoben, Austria, 15. 3. 2013
- Naima Benyagoub, Magali Leger, Prof. Marc Lethiecq, Prof. Franck Levassort, Université François Rabelais, Tours, France, 24.–29. 3. 2013
- Dr. Marko Budimir, Institute for Nuclear Technology-INETEC, Zagreb, Croatia, 13. 5. 2013
- Prof. Jürgen Rödel, Technische Universität Darmstadt, Darmstadt, Germany, 16.–17. 5. 2013
- 12. Prof. Klaus Reichmann, Graz University of Technology, Graz, Austria, 17. 5. 2013
- 13. Prof. Angus I. Kingon, Brown University, Rhode Island, USA, 9.-17. 6. 2013

- 14. Goran Mišković, Vienna University of Technology, Institute of Sensor and Actuator Systems, Wienna, Austria, 13. 6. 2013
- Dr. Vassilios Binas, Foundation for Research & Technology Hellas (FORTH), Institute for Electronic Structure and Laser (IESL), Crete, Greece, 8.-25. 9. 2013
- 16. Dr. Gregor Trefalt, University of Geneva, Geneva, Switzerland, 9.-13. 9. 2013

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- 16. Jitka Hreščak, B. Sc.
- 17. Evgeniya Khomyakova, B. Sc.

BIBLIOGRAPHY

- 17. Prof. Raul Bermejo, Institut für Struktur-und Funktionskeramik, Montanuniversität Leoben, Leoben, Austria, 22.-23. 9. 2013
- Prof. Mariuca Gartner, Prof. dr. Maria Zaharescu, "Ilie Murgulescu" Institute of Physical 18 Chemistry of Romanian Academy, Bucharest, Romania, 4.-8. 11. 2013
- 19. Alja Kupec, B. Sc. 20. Oleksandr Noshchenko, B. Sc. 21. Jernej Pavlič, B. Sc. 22. Tania Pečnik, B. Sc. 23. Jerca Praprotnik, B. Sc. 24. Marko Vrabeli, B. Sc **Technical officers** 25. Darko Belavič*, B. Sc. 26. Andraž Bradeško, B. Sc. 27 Jena Cilenšek, B. Sc. 28. Silvo Drnovšek, B. Sc. 29. Brigita Kmet, B. Sc. 30. Milena Pajić, B. Sc., left 01.05.13 Technical and administrative staff

18. Dr. Jurij Koruza, left 01.08.13

31. Tina Ručigaj, B. Sc.

Note: part-time JSI member

ORIGINAL ARTICLE

- 1. Ilze Aulika, Silvana Mergan, Andreja Benčan, Q. Zhang, Alexandr Dejneka, Marija Kosec, K. Kundzins, D. Demarchi, P. Civera, "Impact of crystallisation processes on depth profile formation in solgel PbZr0.52Ti0.48O3 thin films", Advances in applied ceramics, vol. 112, issue 1, pp. 55-58, 2013.
- 2. Darko Belavič, Marko Hrovat, Gregor Dolanc, Kostja Makarovič, Marina Santo-Zarnik, "Design and fabrication of an LTCC structure for a microceramic combustor: invited paper", J. microelectron. electron. packag., vol. 9, no. 3, pp. 120-125, 2013.
- 3. N. Bensemma, Gregor Trefalt, Sebastjan Glinšek, Marija Kosec, K. Taíbi, M. Abbaci, "Investigation of the $BaTiO_3BaMg_{1/3}Nb_{2/3}O_3$ system estructural, dielectric, ferroelectric and electromechanical studies", Journal of electroceramics, vol. 30, no. 4, pp. 206-212, 2013.
- 4. Vid Bobnar, Hana Uršič, Goran Casar, Silvo Drnovšek, "Distinctive contributions to dielectric response of relaxor ferroelectric lead scandium niobate ceramic system", Phys. status solidi, b Basic res., vol. 250, no. 10, pp. 2232-2236, 2013.
- 5. Goran Casar, Xinyu Li, Jurij Koruza, Qiming M. Zhang, Vid Bobnar, "Electrical and thermal properties of vinylidene fluoridetrifluoroethylene-based polymer system with coexisting ferroelectric and relaxor states", J. Mater. Sci., vol. 48, no. 22, pp. 7920-7926, 2013.
- 6. Jovana Ćirković, Katarina Vojisavljević, Maja Šćepanović, Aleksander Rečnik, Goran Branković, Zorica Branković, Tatjana Srećković, "Hydrothermally assisted complex polymerization method for barium strontium titanate powder synthesis", J. sol-gel sci. technol., vol. 65, issue 2, pp. 121-129, 2013.
- 7. Jitka Hreščak, Andreja Benčan, Tadej Rojac, Barbara Malič, "The influence of different niobium pentoxide precursors on the solidstatesynthesis of potassium sodium niobate", J. Eur. Ceram. Soc., vol. 33, issue 15-16, pp. 3065-3075, 2013.
- 8. Alja Kupec, Pascale Gemeiner, Brahim Dkhil, Barbara Malič, "Phase transitional behavior of potassium sodium niobate thin films", Thin solid films, vol. 539, pp.317-322, 2013.
- 9. Danjela Kuščer, Tina Bakarič, Bojan Kozlevčar, Marija Kosec, "Interactions between lead-zirconate titanate, polyacrylic acid, and polyvinyl butyral in ethanol and their influence on electrophoretic

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- 10. Danjela Kuščer, Oleksandr Noshchenko, Hana Uršič, Barbara Malič, "Piezoelectric properties of ink-jetprinted lead zirconate titanate thick films confirmed by piezoresponse force microscopy", J. Am. Ceram. Soc., vol. 96, no. 9, pp. 2714-2717, 2013.
- 11. Kostja Makarovič, Andreja Benčan, Marko Hrovat, Janez Holc, Barbara Malič, Marija Kosec, Raúl Bermejo, Irina Kraleva, "The effect of phase composition on the mechanical properties of LTCC material", International journal of applied ceramic technology, vol. 10, issue 3, pp. 449-457.2013.
- 12. Kostja Makarovič, Anton Meden, Marko Hrovat, Darko Belavič, Janez Holc, Marija Kosec, "Non-destructive quantitative phase analysis of an LTCC material", Microelectron. int., vol. 30, no. 2, pp. 73-76, 2013.
- 13. Matejka Podlogar, Damjan Vengust, Jacob J. Richardson, Martin Strojnik, Matjaž Mazaj, Gregor Trefalt, Nina Daneu, Aleksander Rečnik, Slavko Bernik, "Parametric study of seed-layer formation for lowtemperature hydrothermal growth of highly oriented ZnO films on glass substrates", Phys. status solidi, A Appl. mater. sci., vol. 210, issue 6, pp. 1083-1092, 2013.
- 14. Jürgen Rödel, Yo-Han Seo, Andreja Benčan, Barbara Malič, Marija Kosec, Kyle Webber, "R-curves in transformation toughened lead zirconate titanate", Eng. fract. mech., vol. 100, pp. 86-91, 2013.
- 15. Brigita Rožič, Marko Jagodič, Sašo Gyergyek, Zvonko Jagličić, Samo Kralj, Vassilios Tzitzios, George Cordoyiannis, Zdravko Kutnjak, "Indirect magnetoelectric coupling in mixtures of magnetite and ferroelectric liquid crystal", In: Proceedings of the ISAF ECAPD PMF 2012, International Symposium on Applications of Ferroelectrics; European Conference on the Applications of Polar Dielectrics; International Symposium Piezoresponse Force Microscopy and Nanoscale Phenomena in Polar Materials, 9-13 of July, 2012, Aveiro, Portugal, Ferroelectrics, vol. 448, no. 1, pp. 12-16, 2013.
- 16. Brigita Rožič, Jurij Koruza, Zdravko Kutnjak, George Cordoviannis, Barbara Malič, Marija Kosec, "The electrocaloric effect in lead-free K_{0.5}Na_{0.5}NbO₃ - SrTiO₃ ceramics", In: Proceedings of the ISAF ECAPD PMF 2012, International Symposium on Applications of Ferroelectrics; European Conference on the Applications of Polar Dielectrics;

International Symposium Piezoresponse Force Microscopy and Nanoscale Phenomena in Polar Materials, 9-13 of July, 2012, Aveiro, Portugal, *Ferroelectrics*, vol. 446, no. 1, pp. 39-35, 2013.

- Marina Santo-Zarnik, Darko Belavič, Vlasta Sedlakova, Josef Sikula, Martin Kopecky, Petr Sedlak, Jiri Majzner, "Comparison of the intrinsic characteristics of LTCC and silicon pressure sensors by means of 1/f noise measurements", *Radioengineering (Prague)*, vol. 22, no. 1, pp. 227-232, 2013.
- Marina Santo-Zarnik, Vlasta Sedlakova, Darko Belavič, Josef Sikula, Jiri Majzner, Petr Sedlak, "Estimation of the long-term stability of piezoresistive LTCC pressure sensors by means of low-frequency noise measurements", *Sens. actuators, A, Phys.*, vol. 199, pp. 334-343, 2013.
- 19. Yo-Han Seo, Daniel J. Franzbach, Jurij Koruza, Andreja Benčan, Barbara Malič, Marija Kosec, Jacob L. Jones, Kyle Webber, "Nonlinear stress-strain behavior and stress-induced phase transitions in soft $Pb(Zr_{1-x}Ti_x)O_3$ at the morphotropic phase boundary", *Phys. rev., B, Condens. matter mater. phys.*, vol. 87, no. 9, pp. 094116-1-094116-11, 2013.
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MENTORING

- 1. Jurij Koruza, *Sintering and phase transition behaviour of sodium niobate:* doctoral dissertation, Ljubljana, 2013 (mentor Barbara Malič; co-mentor Tadej Rojac).
- 2. Kostja Makarovič, *The effect of processing conditions on the phase composition, structure and properties of low temperature co-fired ceramics:* doctoral dissertation, Ljubljana, 2013 (mentor Andreja Benčan Golob; co-mentor Barbara Malič).

ENGINEERING CERAMICS DEPARTMENT

K-6

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

Akin to previous years, in 2013 the investigation of AlN powder hydrolysis in diluted aqueous suspensions was continued. The established mechanistic model for aluminium hydroxide formation during the hydrolysis in a broad temperature range, i.e., between room temperature and the boiling point of water, which was published in 2012, was implemented with a study at 5 °C. The results revealed that throughout the two-week-long hydrolysis at this temperature the pH value of the suspensions was below 9, indicating the hydrolysis remained in the induction Head: period. In parallel, a remarkably high value of dissolved aluminium species in the aqueous part of the suspension Prof. Tomaž Kosmač



was detected, being an order of magnitude higher at a given pH value than the aqueous AlCl₃ solution. The work was accepted in the Journal of American Ceramic Society. These findings are also being tested in practice, since such supersaturated aluminate solutions could well serve as a new precursor for the precipitation of aluminium hydroxide-based thin films and nano-scaled particles in a procedure that could provide an alternative to the well-known sol-gel method.

In the field of electrically conductive ceramic composites we continued the research on the synthesis and properties of composites based on zirconia (Y-TZP) with dispersed titanium nitride (TiN) particles that could be machined with electrical-discharge machining. $\rm ZrO_{s}/\rm TiN$ electro-conductive ceramic composites with various compositions were prepared by two approaches: the mixing of commercial powders and by in-situ precipitation (thermal hydrolysis), which under appropriate conditions enables the homogeneous distribution of TiN particles. The influence of parameters such as temperature, boiling time and pH on the crystallinity, polymorphic modification and size of the synthesized particles was investigated. Some effort was also invested into a study of the sintering behaviour of composites. A homogeneous powder mixture ZrO₂/TiN was prepared by the controlled precipitation of titanium oxide followed by calcination of the obtained powder mixture to titanium nitride by a thermochemical treatment (nitridation). The obtained powder mixture was densified with spark plasma sintering (SPS) to produce dense composites. The impact of the quantity and size distribution of the conducting phase on the concentration, density and electrical conductivity was further investigated. Moreover, the impact of the content and size of the conductive particles on the densification process and the final mechanical and electrical properties of the composites was also studied.

The research on the synthesis of electrically conductive ceramic composites based on silicon nitride was also re-initiated. Previously prepared Si₂N₄ powders coated with TiN or ZrN nanoparticles were this time sintered using the SPS technique. Since this method allows very high heating rates and fast densification compared to conventional sintering we wanted to show that it is possible to hinder the nanoparticles' growth, which was not possible before.

In 2013 the research on self-healing ceramic composites based on silicon nitride/silicon carbide composites was started. The silicon nitride ceramics with dispersed SiC nanoparticles was prepared by mixing the Si₂N₄ powder with polycarbosilane polymeric ceramic precursor, which forms SiC after terms of pore packing.

Prof Tomaž Kosmač was a co-editior of the book Advanced Ceramics for Dentistry, issued in 2013 by Elsevier. The authors of many chapters were from the Engineering Ceramics department and other departments from the Jožef Stefan Institute.



Figure 1: Scanning electron micrographs (SEM) showing the densification of mesoporous ZrO, with hierarchical heterogeneities in



Figure 2: TEM micrograph of zirconia powder coated with TiN nanoparticles used for the preparation of electrically conductive engineering ceramics.

pyrolysis. The powders were successfully densified using SPS, while the size of the SiC particles remained on the nanoscale. These materials exhibit better oxidation properties (and possible self-healing ability) compared to conventionally prepared Si_3N_4 /SiC composites.

In the field of research on dental ceramics we continued by addressing some of the major problems concerning the production of full-ceramic dental contours with tetragonal zirconia (Y-TZP) as a core material, their cementation and their behaviour in clinical conditions. The work was conducted in close co-operation with the Department of Oral Medicine, Medical Faculty at the University of Ljubljana. In particular, we were interested in the role of phase partitioning within the grains, as well as that of stresses caused by the incorporation of aliovalent impurities on the grain boundaries, in the nucleation and growth of the monoclinic laths in the initial stage of ageing. In addition, accelerated ageing experiments with zirconia strips permanently loaded in bending during autoclaving were conducted in order to evaluate the influence of external stresses on the kinetics of the transformation during accelerated ageing. The combined effect of silica and alumina on the ageing resistance and mechanical properties of 3Y-TZP ceramics was evaluated. Specimens were prepared by the infiltration of a silica sol into the pre-sintered porous 3Y-TZP pellets, produced from commercially available powders, containing different amounts of alumina (0.05 and 0.25 wt. %). It

was found that the presence of silica in alumina-free 3Y-TZP greatly increases the resistance to ageing. The addition of small amounts of silica to alumina-containing 3Y-TZP further improves the ageing properties of t-zirconia, due to a possible distinctive mechanism of suppression, without affecting the flexural strength, Vickers hardness and indentation toughness. Finally, an in-vivo study aimed at monitoring the propagation of the t-m transformation of high-translucency 3Y-TZP ceramics directly exposed to the aggressive environment of the oral cavity in the absence of an externally applied stress has been started. Namely, according to most follow-up studies performed so far, the main reason for the repair or replacement of all-ceramic fixed partial dentures (FPDs) is porcelain chipping, which occurs much more frequently than the chipping of porcelain bonded to metal-ceramic FPDs. Since none of the numerous engineering concepts pursued worldwide in order to overcome the chipping problem proved to be sufficiently effective, an ever-larger number of frustrated clinicians is gearing towards porcelain-free crowns

We have developed a novel method for the preparation of β-TCP coatings on ceramic bone implants with tailored physico-chemical properties, i.e., surface topography, mechanical strength and dissolution rate.

and bridges. In our experiment, sintered zirconia discs, differing in their composition, microstructure and surface treatment, were implanted in the lingual flange of the lower dentures to be worn by recruited edentulous patients from the Department of Prosthodontics, Medical faculty, University of Ljubljana. After every 6 months the discs will be explanted, gently cleaned by ultrasonication to remove the adhered proteins and subjected to XRD and FE-SEM surface analyses. In order to evaluate the durability and reliability of "high translucent" Y-TZP ceramic, a series of full-anatomic four-unit poste-

rior bridges was designed and soft-milled from commercially available zirconia blanks using a conventional CAD/ CAM technique and sintered under different conditions (heating/cooling rate, end temperature, dwell time) to produce materials differing in the microstructure-related properties (damage tolerance, ageing behaviour). After glazing, they were subjected to mechanical fatigue testing under simulated clinical conditions. We were interested in compromise solutions between aesthetic design (thickness of the abutments and their transition to connectors) and durability for materials differing in sintering conditions and surface treatment. The results will be used in the material selection and denture design in the Department of Oral Medicine, University of Ljubljana. Yet another clinical testing has started in 2013 involving the surface functionalization of sintered zirconia by applying nanostructured adhesive coatings in a non-invasive process that has been recently developed in our group. The following two types of dentures were deemed most appropriate for the verification of nanostructured adhesive coatings in practice, because their long-term survival rate to a large extent depends on the adhesive bond strength and a stronger bonding than currently achievable would be very advantageous. These are: three-unit inlay-retained bridges replacing missing single premolars and molars that have become increasingly popular due to the conservative approach to prosthetic rehabilitation, and conical primary crowns supporting secondary galvano-crowns of removable partial dentures. Here again, volunteers were recruited among patients from the Department of Prosthodontics, Medical faculty, University of Ljubljana.

In 2013 dr. Andraž Kocjan ended his post-doctoral training at Stockholm University, where he was employed as a guest researcher. He was studying the processing and sintering of mesoporous zirconia (ZrO_2) ceramic powder. In the scope of this investigation his project entitled "*Improved Reliability of Translucent Dental Zirconia and*"

Alumina Ceramics" was chosen and financed through a call - Frontiers of Research 2012 (JECS Trust foundation). The aim of the project was to prepare reliable and translucent ZrO₂ dental ceramics for full-contour dental restorations with no porcelain overlay. The project was successfully finalized and the results presented with an oral presentation entitled *"Processing of Advanced (Dental) Zirconia Ceramics*" at the ECERS XIII conference (Limoges, France). Parts of these results were published in the *Journal of European Ceramic Society*.

With the defence of a doctoral dissertation the research on the synthesis of bioactive calcium phosphate coatings on zirconia Y-TZP ceramics was successfully completed. The Y-TZP ceramics are frequently used in medicine as a material for dental implants due to their aesthetical and mechanical properties. The fixation of an implant can be improved as its surface is covered by bioactive calcium phosphate coating that forms a strong bond with bone tissue. The coatings were prepared using a biomimetic method in which the ceramic substrate is immersed in a solution with the same physiological temperature and similar composition as human blood plasma. The advantages of this bio-mimetic method are its simplicity, low price and good



Figure 3: A general examination of the fracture surface using the optical microscope and by adjusting the lighting indicated that the fracture progressed as shown by the arrows.

control of the composition of the coatings. One of the main problems that restrict the use of bio-mimetic coatings in medicine is the poor adhesion of the coatings to the substrate, so in the research we primarily dealt with ways of improving the mechanical properties of the coatings. It was found that the thermal treatment improved the adhesion of the coatings and at the same time it enables us the control of their phase composition. Thus, we have developed

procedures for the synthesis of calcium phosphate coatings with different - phase composition (hydroxyapatite, octacalcium phosphate), β -tricalcium phosphate), different morphology and mechanical properties. The procedure was described in an article published in the *Journal of European Ceramic*

In 2013 we cooperated with research institutions and industrial partners.

Society. Especially important is a new procedure for the synthesis of thin β -tricalcium phosphate coatings with very good mechanical properties. Mechanical tests showed that the adhesion of such coatings is comparable or even better than the adhesion of calcium phosphate coatings on commercially available bone grafts.

In the frame of the research on thermoplastic ceramic suspensions the new one-step thermal process for the removal of the binder from a low-pressure injection-moulded part and subsequent sintering was developed. This was done using high-purity carbon, since it enables the extraction of the binder from the samples and is afterwards burned out during the subsequent sintering process, which enables one-step thermal processing of the samples. The research was published in the *Ceramics International* journal.

Wit the company Hidria AET d.o.o. from Tolmin we cooperated in the field of maintenance and operational work in the field of centreless grinding of technical ceramics. We also cooperated with Institute of Ecological research ERICo in the field of the analysis of the particle size and distribution of materials that are transported to and from Luka Koper.

Some outstanding publications in the past three years

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INTERNATIONAL PROJECTS

Services 1. Foreign buyers

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

Prof. Tomaž Kosmač

RESEARCH PROGRAM

Engineering and Bio-Ceramics Prof. Tomaž Kosmač

R&D GRANTS AND CONTRACTS

Research of Dental Ceramics Prof. Tomaž Kosmač

VISITOR FROM ABROAD

Dr. Vaclav Pouchly, Central European Institute of Technology (CEITEC), Brno University of Technology, Department of Ceramics and Polymers, Brno, Czech Republic, 19.8.-20.11.2013

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LECTURE)

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DEPARTMENT FOR NANOSTRUCTURED MATERIALS K-7

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

In 2013 we began work on the EU FP7 project "Nanocrystalline permanent magnets based on hybrid metalferrites" (NANOPYME). Our role is as the developer of 100-nanometer-scale Sr-ferrite particles via high-energy ball milling, with subsequent activities in the project related to the consolidation of two-phase exchange-coupled materials and the transfer of the process to the industrial partners, including Magneti Ljubljana d.d., during the final year of the project. The first 6-month meeting was held in Ljubljana during the last week of May 2013.



In the frame of ARRS-funded project "The protection of permanent magnets for advanced applications at high Head: temperatures" we designed and developed an effective coating for magnets used at temperatures in the range of **Prof. Spomenka Kobe**

400 °C. Multilayer coatings based on nickel and titanium nitride are proving to be very effective at these very high temperatures, resisting both corrosion and evaporation.

In another study, the so-called grain-boundary diffusion process (GBDP) was introduced. This is a post-sintering process, where the diffusion of Dy or Tb along grain-boundaries and into the outer parts of Nd₂Fe₄B grains occurs and this contributes to a higher coercivity. The result is a "core-shell" microstructure where the core is represented by the Dy-free Nd₂Fe₄B phase and the shell is rich in Dy (NdDyFe₁₄B). The first step that is needed in such a process is to coat the commercially available, Dy-free Nd-Fe-B sintered magnet with Dy-powder, in our case DyF₃. The magnets were coated in two different ways. The first is by dip-coating and the second is by the more efficient electrophoretic deposition (EPD). The grain size of the DyF,-powder was in range of $5 \,\mu\text{m}$ to $60 \,\mu\text{m}$ and the suspension was based on ethanol. In the case of using EPD, the thickness of the DyF₂-coating was varied from a few to 250 µm. After the coating-process, all the magnets were usually exposed to the same heat treatment at 850 °C for 10 hours and aging at 500 °C for 1 hour in an argon atmosphere. In this step, the so-called GBDP occurs. The magnetic measurements of such magnets were made with a permeameter. When rough calculations were made, to figure out how high is the Dy-concentration after GBDP, it was determined that in a whole magnet there is less than 1 wt. % of Dy and magnetic properties are even better or as good as in the case of magnet produced by the conventional powder metallurgy route that contain 2 wt. % of Dy. For this reason, GBDP based on EPD is an extremely attractive process that leads to a large coercivity improvement (up to 30 %) with only small drop in remanence. This work is part of the European project ROMEO (FP7-NMP-2012-SMALL-6) where one of the main goals is to reduce the usage of expensive heavy rare earths (Dy or Tb) in the NdFeB magnets and at the same time retain or even enhance the magnetic properties.

The deposition process of the Fe-Pd nanostructured alloys was kinetically evaluated and the parameters for an optimum composition depending on the system investigated, i.e., Fe₇₀Pd₂₀ or Fe₅₀Pd₅₀ was given. Magnetic shape memory $Fe_{70}Pd_{30}$ nanorods, which we are investigating in the frame of a national project with NIC and an MNT-ERA-NET project, were successfully deposited in a narrow composition range. Low-temperature SQUID measurements showed an increased magnetization saturation and coercivity, Jeol 2100).

In October 2013 we began coordinating a new EU FP7 project called "New permanent magnets for electric-vehicle drive applications" (MAG-DRIVE) to develop new processing technologies for rare-earth transition-metal magnets that will be incorporated into electric motors with higher efficiency. The project includes partners from the UK, Germany, Serbia, France and Slovenia. At the JSI, as well as coordinating the project we will be working on innovative compaction techniques such as spark-plasma sintering in an attempt to improve the magnetic properties by reducing as far as possible the grain growth inherent in high-temperature consolidation



Figure 1: Agglomerates of mackinawite (FeS) leaves with corresponding experimental and simulated EDP. Individual mackinawite crystal with a mechanism of Cu incorporation between the mackinawite layers (TEM

processes.

Fe-Pd nanorods were successfully implemented in xerogels together with a model drug. The biocompatibility of the system was proven with an in-vivo experiment involving zebra fish. In the $Fe_{50}Pd_{50}$ nanorod system homogenous nanowires were deposited. A low magnetocrystalline phase in the as-deposited state was converted to the highly anisotropic L1_o structure, exhibiting high coercivities Hc = 128kA/m. implying a transformation from a high-temperature austenite cubic phase to a low-temperature tetragonal martensitic phase. The magnetization distribution in FePd single nanowires was found in a single domain state with the preferential easy axis of the magnetization orientated in a parallel direction to the wires; however, the magnetization easy axis in an FePd nanowire array was found to be in the perpendicular direction, due to the expressed dipole-dipole interactions. On the other hand, Co-Pt nanowires of the same morphology exhibited a unique quasi-periodic magnetization distribution due to the anisotropy interplay between the shape anisotropy and the two crystalline anisotropies originating from the Co-Pt fcc and hcp phases. Such nanowires represent suitable candidates for applications such as race-track memory devices. In the past year we have introduced a new field of multi-

functional FePt-Au core/shell nanostructures suitable for novel magneto-photo medical curing. A suspension of FePt/ SiO₂/Au core/shell nanoparticles in water was irradiated with a laser at the wavelength λ =810nm (P=1W) suitable for curing humans. A significant temperature increment of the media surrounding the nanoparticles was detected. We reported on nitrogen-filled **hollow Co-Pt nanospheres** produced via pulsed-laser ablation (PLA) in ambient nitrogen gas. In this study we have demonstrated that by applying PLA in an ambient nitrogen gas the gas-filled

hollow Co-Pt nanospheres can be successfully produced, where the composition of the particles is controlled by the



Figure 2: High-resolution FEGSEM micrograph of the Fe-Pd nanorods with superimposed diagram showing the variation of the atomic Fe/ Pd ratio along the nanorod (points 1-10). The results were obtained from optimized low-voltage quantitative elemental EDS analysis with submicrometer analytical spatial resolution.

Co-Pt target composition. By means of various techniques of transmission electron microscopy we aimed to characterize both the structure and the composition of synthesised nanospheres as well as to determine the nitrogen pressure inside the individual voids. The data was further employed for the reconstruction of the formation mechanism of Co-Pt gas-filled nanospheres and the suggestions for the general formation mechanism for gas-filled nanospheres in other metallic systems have been made.

Highly coercive permanent Nd-Fe-B-based magnets were successfully developed from commercially available MQU-F rapidly quenched ribbons with optimized composition by wet coating with DyF_3 in isopropanol and subsequent spark plasma sintering and heat treatment. The highest H_{ci} enhancement was obtained at 2.2 wt.% Dy-fraction, i.e., from 1580 to 2025 kA/m, which is a 25 % improvement. When more than 3 wt.% of Dy was added, the coercivity enhancement started to decrease, whereas at 4.8 wt.% the coercivity of the as-sintered magnet was lower than it was for the non-coated one and it was further decreasing with the annealing time. Based on the SEM results and the thermodynamic data on DyF_3 and NdF_3 formation enthalpies it appears that at a certain DyF_3 content a continuous NdF_3 layer starts to form that prevents Dy diffusion from the ribbons' interfaces. This explains an optimal addition of DyF_4 . This innovative approach of manufacturing

fully dense Nd-Fe-B magnets with enhanced coercivity and a gradient microstructure was patented at the European Patent Office under patent number 1556. The research was performed within the scope of the EU project ROMEO.

We investigated the magnetic exchange interaction on the basis of Wannier orbitals obtained from electronic structure calculated ab initio. The so-determined parameters may be applied in the density-matrix-renormalization-group (DMRG) method, which is efficient mainly for one-dimensional systems. Within the framework of the density-functional theory we explored the possibilities for the presence of non-stabilities and **complexities in the Ca-Ga-Cu phase diagram**. We also determined the influence of beryllium on the twin-boundary energy in spinel.

In 2013 we broadened the research work of structural materials within the frame of the **European fusion programme** from ceramic composites SiC/SiC to tungsten-containing composites. For samples preparation we used the same processing technique as for the SiC/SiC and we investigated the influence of the tungsten content on the properties of the W-Si-C composites in the range of low and high tungsten content. The results have confirmed that by optimisation of the process, a relatively high strength can be achieved in both regions.

One of the important research topics is the **electrophoretic deposition** (EPD) of various materials. Among them, in 2013, the main attention has been paid to silicon carbide, carbon nanotubes and polymer polyether-ether-ketone (PEEK). The highest green densities were achieved from aqueous suspensions with a high solids loading (>40 wt. %) and with the optimal addition of surface-active agents, providing that the electrical conductivity is
limited. Based on a comprehensive study of the deposits and suspensions before and after the deposition we explained the process for forming bulk SiC and PEEK parts.

In collaboration with Mechanical Engineer Faculty, UL, we were also dealing with the preparation of homogeneous PEE composites with nanoparticles (MoS_2 , WS_2 , CNT and graphene). The green parts were densified at various temperatures below and above the melting point and their wear properties were analysed. The results imply a significant influence of the processing temperature.

In the frame of the **project BioTiNet** (FP7-ITN) we continued with the analysis of the properties of **anatase** (TiO_2) **coatings**, grown by hydrothermal treatment on titanium alloys for bone-implant applications. In collaboration with the University of Barcelona, we confirmed the improved corrosion resistance of the coated alloys; moreover, we also verified the UV photo-induced properties of nanostructured TiO₂ coatings. The excellent photocatalytic activity of the firmly bonded coatings has been confirmed, as well as the UV photo-induced super-hydrophilicity, which appeared also as a prolonged effect (up to two weeks of recovery). In collaboration with the



Figure 3: Development of (111) twin grains in MgAl2O4 spinel. Until the twin-boundary-forming dopant is available, the grains grow exaggeratedly along this boundary and consequently develop plate-like morphology unusual for the cubic spinel. Subsequently they thicken according to the normal grain growth Ostwald ripening law.

University in Sienna, the effect of the presence of the coating and its pre-irradiation with UV light on plasma protein adsorption have been studied, while in collaboration with the University of Giessen we verified the interaction with human cells. In continuation, the investigation will be completed by the analysis of the proposed bacteriostatic effect after UV pre-irradiation.

The investigations of materials for **biomedical application** involved the preparation and analysis of the scaffolds for hard-tissue engineering that is a topic of the COST action NAMABIO (From nano to macro biomaterials and applications to stem cells regenerative orthopaedic and dental medicine).

Within investigations of n-type oxide thermoelectric materials we synthesized Nb-doped SrTiO₃. The basic microstructure of solid-solution $Sr(Ti_{0.8}Nb_{0.2})O_{3x}$ was modified in two ways: with the addition of $Sr_3Ti_2O_7$ nucleation seeds and/or with the addition of SrO-excess. $Sr_3Ti_2O_7$ seeds were synthesized by molten salt approach. In the case when excess SrO was added to a $Sr(Ti_{0.8}Nb_{0.2})O_{3x}$ solid solution we obtained material that was composed of two phases, namely, $Sr(Ti_{0.8}Nb_{0.2})O_{3x}$ and polytypic Ruddlesden-popper phases. More or less ordered single planar faults with the SrO structure were also observed in the perovskite matrix. Measurements of thermoelectric

We prepared bioactive biodegradable scaffolds from composites of gellan gum reinforced with bioactive-glass nanoparticles, which helped to enhance the microstructure (pore size and interconnectivity), mechanical properties and formation of hydroxyapatite in simulated body fluid. Optimisation of the processing resulted in further improved mechanical properties by a better particles distribution in the polymer matrix and an increased amount of bioactive-glass reinforcement.

properties of so far synthesized materials showed that the achieved a ZT value of approximately 0.12. In the field of oxide thermoelectric materials we studied the influence of the sintering method (pulse electric current sintering – PECS, microwave sintering) and doping with oxides of Al, Mn, Fe, Ce and Nd on the structure, microstructure development and thermoelectric characteristics of ceramics in the system (ZnO) In₂O₄ (k = 5, 11).

Perovskite materials such as SrTiO, nanostructures are suitable for many applications such as oxygen sensing and tunable HTS (high temperature superconducting) microwave filters. The potential advantages of the nanostructured forms have been, however, scarcely explored compared to other oxides. The synthesis of perovskite SrTiO₃ nanostructures via solgel electrophoretic deposition (EPD) into anodic aluminium oxide (AAO) membranes has proven to be very successful and useful. When measuring the electrical properties of SrTiO3 nanotubes we obtained interesting scientific findings, which were published in the journal Materials Chemistry and Physics. In the article titled: "Insight into the structural, electrical and photoresponse properties of individual Fe:SrTiO, nanotubes" we reported on the structural and electrical properties of individual iron-doped strontium titanate nanotubes (Fe:SrTiO₂) grown by electrophoretic deposition (EPD). The Fe:SrTiO₂ nanotubes were assessed for the first time, showing high stability and reproducibility. This result paves the way to the further development of more complex titanate-based devices, as for instance nanostructured oxygen Fe:SrTiO₃ sensors. From the experimental data it was concluded that



Figure 4: Coercivity dependence of spark plasma sintered and annealed MQU-F42 commercial alloy on addition of DyF_3 powder from isopropanol suspension



Figure 5: Cross-section TEM image of seed-layer and initial stages of film growth with illustrated SCOG mechanism. SCOG mechanism is expressed through three distinct growth stages: (i) random nucleation, (ii) spatial confinement, and (iii) oriented growth.

The influence of an organic vehicle and the amount of added varistor powder filler on the rheological characteristics of pastes and their screen-printing performance was studied. A paste with high solids load of 70% and good printing characteristics was developed and enables preparation of dense layers of varistor ceramics with good electrical characteristics at low sintering temperature of 900 °C, typical for the screen-printing hybrid circuit technology. the polycrystalline form of Fe:SrTiO₃ nanotubes is the major limitation to attain high photoconductivity gains when exposed to UV-light.

We optimized parameters for the anodization of aluminium alloys. The obtained oxide layer was coloured by selected ion. In the case of copper ions we obtained a purple colour of oxide layer. This work was performed in cooperation with the department of thin films and surfaces (F3) and Impol industry.

In the field of **dye-sensitized solar cells** (DSSCs) we focused our research on the fabrication of high-efficient photo-anodes composed of TiO_2 nanotubes. A self-ordered, vertically aligned TiO_2 nanotubes, were grown on electropolished titanium foil by anodic oxidation in viscous organic electrolyte. By changing the anodization parameters (temperature, time, applied voltage, electrolyte composition) TiO_2 nanotube arrays with different morphologies were obtained. Some of the TiO_2 nanotubes were additionally treated with TiCl_4 or with TiO_2 P25. The prepared photo-anodes were assembled into flexible and nonflexible DSSCs. Measured current-voltage characteristics showed that the maximum energy conversion efficiency for flexible DSSCs was 2.1% and for nonflexible 5.9%.

We developed homogeneous coarse-grained low-voltage **ZnO-based** varistor ceramics doped with Bi₄Ti₃O₁₂ or Bi₁₂TiO₂₀ and other varistor dopants having breakdown voltage in the range from 20 to 40V/mm and nonlinearity coefficient α above 20. The development was based on the discovery that rapid decomposition of pre-reacted phases from the Bi₂O₃TiO₂ system into TiO₂-rich Bi₂O₃ liquid phase enhances formation of inversion boundaries in the ZnO grains, which results in homogeneous grain growth and microstructure development.

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

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



Figure 6: Left - meteorite Jezersko (mass 1380 g) Right - Typical barred olivine chondrule observed in cross-polarized light



In the field of **photocatalysis** we designed and fabricated Ti-foil based microreactor with titania nanotubes and anatase nanoparticles. Basic photocatalytic properties and design was published in ACS applied materials & interfaces (IF 5). Using this microreactor we performed series of experiments where we studied the mechanisms of degradation reactions for

various types of organic substances. It was found that during the decomposition of organics containing chlorine the efficiency of the microreactor seriously decreased. With EPR measurements we tried to establish the mechanism of this phenomena, namely the chlorine could adsorb on the surface of nano-anatase particles and due to steric effects hindered the adsorption of the organic molecules or could produce chlorine radicals which are concurrent

to hydroxyl radicals. The photocatalysis of zinc oxide as a function of crystallinity and particle size was also studied and published in Applied Catalysis. B, Environmental (IF 5,8).

Self-assembly of Ge, Ni and Co quantum dots in amorphous silica matrix after the high-energy ions irradiation was investigated using electron microscopy and microanalysis. With co-workers we published series of 4 papers on self-organization of quantum dots. With the synthesis parameters we were able to prepare different superstructures. In collaboration with scientists from Portugal the influence of carbon nano-tubes addition to TiO, and morphologies if titania on photocatalytical degradation of caffeine were explained in papers published in Catalysis Today.

We synthesized and further investigated Cu-doped Fe-sulphides. With electron microscopy, X-Ray diffraction and magnetic measurements we showed the influence of copper on the first precipitate and on the subsequent phase transformations in FeS system. TEM investigation of Cu-doped mackinawite-like FeS showed enhanced crystallinity accompanied with expansion of the unit cell along the c-axis, proportional to the amount of Cu adsorbed between the (001) layers of the mackinawite structure. The subsequent solvothermal treatment and sulphurization of undoped FeS resulted in formation of pyrite, at low doping Cu-rich mackinawite and cubic (Fe,Cu)S with a sphalerite-type structure were formed, while at higher Cu concentrations the end-products were chalcopyrite and bornite, corresponding to the initial amount of Cu in the reagents. These mackinawite properties can be also used for sorption of Cu, Ni or Cr from degraded environment. The results of work were published in two scientific articles.

In the frame of the basic research project 'Twinning, epitaxies and phase transformations in minerals' we continued with nanostructural investigations of growth-type transformational defects in different systems. In the

spinel-chrysoberyl system we confirmed our hypothesis that twinning in MgAl₂O₄ spinel is triggered by the addition of BeO. The results of this work are published in CrystEngComm (IF 3.879). In the rutile-hematite system we studied the mechanism of topotaxial transformation of ilmenite to rutile and hematite. These minerals are related through a common close-packed oxygen sublattice. While ilmenite and hematite have a rhombohedral symmetry, the rutile lattice is slightly tetragonally distorted. Under certain conditions, ilmenite transforms (oxidises) to rutile and hematite, where rutile lamellas precipitate along structurally defined crystal planes of the precursor and finally form reticulated network also known as sagenite. The products of ilmenite oxidation are common in nature and the reaction is also of technological importance for the production of rutile from ilmenite precursor. In the previous year we finished a study of topotaxial rutile-hematite intergowths from the locality Mwinilunga in Zambia, where we determined the crystal-

lographic relationship between rutile and hematite and suggested a mechanism of their formation based on an extensive transmission electron microscopy study. A manuscript for the journal 'Contributions to Mineralogy and Petrology' is in preparation. In addition we started a detailed study of the ilmenite to rutile/hematite transformation mechanism at the atomic level. For this purpose we performed thermal or hydrothermal treatment of natural single crystals of ilmenite. The results show that different transformation mechanism exists based on the treatment technique. During hydrothermal treatment, transformation is based on the dissolution-precipitation mechanism, while during thermal treatment; the recrystallisation is based on the internal rearrangement of atomic within the rigid oxygen sublattice.

Up to date three meteorites have been found on the territory of Slovenia, one stony and two iron types. The highly conserved stone meteorite named after the location Jezersko has recently joined to the collection of Slovenian meteorites. The detailed studies of the meteorite Jezersko, which were performed jointly at the Jožef Stefan Institute, Geological Survey of Slovenia, Faculty of Natural Sciences and the Museum for Natural History of Slovenia offers us an unique opportunity for in-depth understanding of the origin and evolution of our solar system in the last \sim 4.6 billion years. Meteorite Jezersko was registered into the database of all known meteorites in Lunar and Planetary Institute (Meteoritical Bulletin Database).

Within the ARRS project J2-4237 we have investigated the innovative materials using advanced methods of high-resolution scanning electron microscopy (FEGSEM) and quantitative elemental analyses by energy-dispersive and wavelength-dispersive X-ray spectroscopies (EDS, WDS). These methods were modified and improved for reliable materials characterization on submicrometer and nanometre-scale. Using the electron backscatter diffraction (EBSD) analysis we have investigated the crystallinity and the presence of quasicrystals in complex metallic alloys based on Al and Gd-Cu-Ca.

For industrial partners and other research institutions we have performed the analyses and Figure 7: Schematic presentation of photocatalytic expertise related to microstructural characterization of various materials which were included in *microreactor and its design and fabrication*

We successfully synthesised simple and complex twins of spinel, which proved that the ccp-hcp transformation is caused by the presence of beryllium at the (111) twin boundaries. At higher BeO additions we observed the formation of epitaxial overgrowths of spinel with BeMg₃Al₈O₁₆ taaffeite-type compounds. This finding has a potential applicative value since twinned spinel grains develop a plate-like morphology that may improve the mechanical properties of spinelbased ceramics.



Members of the department have also been active in the promotion of science. In 2013 we presented some of the achievements in the TV programme "Bite the Science". Under the umbrella of the Slovenian Society for Science and Engineering (SATENA) we organised the first two sets of popular lectures on science for general public ("Science on the street, knowledge and ideas on the go". the research and development of new products. Main collaborations were realized with SwatyComet Maribor, Cinkarna Celje, Belinka Ljubljana, UL-NTF Department of Materials and Metallurgy, Ljubljana, RC SIMIT Kidričevo, Ortopedska Bolnišnica Valdoltra Ankaran.

One of the important research areas of the group is the implementation of various electron microscopy analytical techniques within the existing EU project ESTEEM2, such as electron energy-loss spectroscopy (EELS), highresolution scanning transmission electron microscopy (STEM, HAADF-STEM) electron holography and mechanical preparation of the TEM samples. The research group is additionally strongly involved in managing of the Center for Electron Microscopy within the frame of the National Infrastructure Center

for microstructural and surface analysis. Implementation of various electron microscopy analytical techniques and the possibility for researchers to access research infrastructure for electron microscopy is of utmost importance for numerous research institutions, industrial partners, as well as for graduate and post-graduate education.

Awards and appointments

- Saša Novak Krmpotič, State (Zois) recognition of scientific achievements in the field of materials, Ljubljana, 22. 11. 2013
- Nina Kostevšek, Kristina Žužek Rožman, Sašo Šturm, Spomenka Kobe, "Hybrid FePt/Au Nanoparticles With a Combined Magneto-Photothermal Effect", The best presentation among young researchers in the research field Nanomaterials and Nanotechnology, 21st Conference on Materials and Technology, Portorož, Slovenia, 13.–15. 11. 2013
- Marja Jerič, Miran Čeh, "Molten salt synthesis of Nb-doped Sr₃Ti₂O₇ platelet seeds", The best poster among young researchers in the research field Nanomaterials and Nanotechnology, 21st Conference on Materials and Technology, Portorož, Slovenia, 13.–15. 11. 2013
- 4. Medeja Gec, Matic Krivec, Kristina Žagar, Luka Suhadolnik, Darja Jenko, Goran Dražić, Miran Čeh, "Comparison of TEM lamella preparation techniques on titania nanotube-arrays/metal Ti interface", MC2013 Best poster award in Instrumentation and Methods, at the MC2013 Microscopy Conference, Regensburg, Germany, 25.–30. 8. 2013
- Sandra Drev, Aleksander Rečnik, Nina Daneu, "Twinning and inclusions in chrysoberyl from Pratinhas, Brazil", MC2013 Best poster award in Materials scince at the MC2013 Microscopy Conference, Regensburg, Germany, 25.–30. 8. 2013

Organization of conferences, congresses and meetings

- 1. 1st CalGadX Conference, Ljubljana, Slovenia, 12.–13. 12. 2013
- 2. 21st International Conference on materials and Technologies, Portorož, Slovenia, 13.–15. 11. 2013 (coorganisation)
- 3. C-MAC Days 2013, Ljubljana, Slovenia, 9.–12. 12. 2013 (members of Science Board and General Assembly in European integrated Center for the Development of New Metalic Alloys and Compounds (C-MAC))
- 4. EMAS 2013, 13th European Workshop on Modern Developments and Applications in Microbeam Analysis Porto, Portugal, 14.–18. 5. 2013 (members of Managing Board of European Microbeam Analysis Society)
- 5. Microscopy Conference 2013, MCM2013, Regensburg, Germany, 25.–30. 8. 2013 (members of International Advisory Board)
- 6. Fusion Expo: The Big Bang, UK Young Scientists & Engineers Fair, London, United Kingdom, 14.–17. 3. 2013 (co-organisation)
- 7. Fusion Hands on experiments at ECSITE Annual Conference, Gothenburg, Sweeden, 6.-8. 6. 2013 (coorganisation)
- 8. Fusion Expo: Science Days 2013, Rust, Germany, 10.-12. 10. 2013 (co-organisation)
- 9. Fusion Expo: Scientific Festival Week of Science and Technology 2013, Prague, Czech Republic, 1.–15. 11. 2013 (co-organisation)
- 10. Fusion Expo: Campus Drie Eiken, Antwerpen, Belgium, 21.-22. 11., 26.-27. 11. 2013 (co-organisation)

INTERNATIONAL PROJECTS

- 1. Services for the Exports Foreign Clients
 - Dr. Zoran Samardžija
- 7FP MACAN; Merging Atomistic and Continuum Analysis of Nanometer Length-scale Metal-oxide Systems for Energy and Catalysis Applications European Commission Asst. Prof. Aleksander Rečnik
- 7FP 2020 Interface; Nanoscale of Tribological Interfaces for Clean and Energy-Efficient Diesel and Gasoline Power Trains
- European Commission
- Asst. Prof. Matej Andrej Komelj
- 4. 7FP BioTiNet; Academic-Industrial Initial Training network on Innovative Biocompatible Titanium-based Structures for Orthopaedics European Commission
 - Prof. Spomenka Kobe
- 5. 7FP ESTEEM 2; Enabling Science and Technology through European Electron Microscopy
 - European Commission Prof. Miran Čeh
- 7FP NANOPYME; Nanocrystalline Permanent Magnets Based on Hybrid Metal-Ferrites European Commission
- Asst. Prof. Paul John McGuiness
- 7FP Fusion Expo; Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN-FUSEX Ministry of Education, Science and Sport
 - Asst. Prof. Saša Novak Krmpotič
- 7FP EURATOM; Review R&D on Materials 4.1.1.2., WP11-DAS-MAT-M03-01/MHEST/PS Ministry of Education, Science and Sport Asst. Prof. Saša Novak Krmpotič
- 7FP ROMEO, Replacement and Original Magnet Engineering Options European Commission
 - Prof. Spomenka Kobe
- 4.1.1.-FU, EURATOM-MHEST; Development of W-Containing Composites Ministry of Education, Science and Sport Asst. Prof. Saša Novak Krmpotič
- 4.1.2.-FU, EURATOM-MHEST; Development of W-Containing Composites Ministry of Education, Science and Sport Asst. Prof. Saša Novak Krmpotič
- 7FF MAG-DRIVE; New Permanent Magnets for Electric-Vehicle Drive Application European Commission
 - Asst. Prof. Paul John McGuiness
- MODEF Creazione e Sperimentazione Congiunta di Modelli per l'Ottimizzazione dell'Utilizzo di Energia Fotovoltaica Unindustria Rovigo
 - Dr. Zoran Samardžija
- COST MP1005, NAMABIO; From Nano to Macro Biomaterials (Design, Processing, Characterization, Modelling) and Applications to Stem Cells Regenerative Orthopedic and Dental Medicine COST Office
 - Asst. Prof. Saša Novak Krmpotič
- Minerals as a Precursors for Advanced Technologies Slovenian Research Agency
 - Asst. Prof. Nina Daneu
- Microstructural Investigation of Materials for Hydrogen Storage and Correlation with Desorption Properties
 - Slovenian Research Agency Asst. Prof. Sašo Šturm
- 17. Experimental and Theoretical Investigation of Hydrogen Sorption in Mg-Zr-Fe-Ni and Ti-Fe-Ni Systems
 - Slovenian Research Agency Dr. Andraž Kocjan
- 18. The CALGAD-X Project: New Calcium-Gadolinium-X Complex Metallic Alloys Slovenian Research Agency
- Prof. Spomenka Kobe
- Study of Chemical Strain in Perovskites Doped With Aliovalent Cations by Applying In-Situ X-Ray Diffraction, Dilatometry and Advanced Transmission Electron Microscopy Techniques Slovenian Research Agency
 - Asst. Prof. Sašo Šturm

RESEARCH PROGRAM

1. Nanostructured Materials Prof. Spomenka Kobe

R&D GRANTS AND CONTRACTS

- 1. New Metallic Materials for Thermal Storage of Digital Information Dr. Andraž Kocjan
- Near-net Shape Nanoparticle-Reinforced Polymer-Composites for Highly-Loaded Advanced Mechanical Components with Superior Tribological Performance Asst. Prof. Saša Novak Krmpotič
- Novel Functionalized Nanomaterials for Applications as Nano- or Biosensors/Actuators/ Bioresponsive (Carrier) Systems
- Asst. Prof. Kristina Žužek Rožman 4. Twinning, Epitaxy and Phase Transformations in Minerals
- Asst. Prof. Nina Daneu
- Electron Microscopy and Microanalysis of Materials on Submicrometer scale Dr. Zoran Samardžija
- 6. Hydrothermal Synthesis of Strongly Adhered TiO2 Photocatalytic Coatings on Metallic Substrates
- Asst. Prof. Goran Dražić 7. Microbial Adhesion Management on Material Surfaces
- Asst. Prof. Goran Dražić B. Development of the Model of the System for Intelligent Support of the Selection of Suitable Powder Material when Developing Sintered Products
- Asst. Prof. Saša Novak Krmpotič 9. Modification of TiO2 Nanoparticle Surface: Prevention of Agglomeration and Preservation of Intrinsic Properties
- Asst. Prof. Aleksander Rečnik 10. Innovative Production Systems for Vaccines and Regenerative Medicine Asst. Prof. Aleksander Rečnik
- 11. High-coercivity Nd-Fe-B Bonded Magnets for Automotive Applications Prof. Spomenka Kobe
- 12. Protected Permanent Magnets for Advanced High-Temperature Applications Asst. Prof. Paul John McGuiness
- Materials and Technologies for Applications of ZnO-based Thick Film Varistors and Oxide Thermoelectrics Asst. Prof. Slavko Bernik
- Colour, Absorption and Protective Nanolayer Coatings for Aluminium alloy Prof. Miran Čeh
- 15. NSFM: Novel Smart Filtration Media Asst. Prof. Kristina Žužek Rožman
- Advanced Methods and Technologies for Processing of a New Generation of ZnO-based Varistor Ceramics
- Asst. Prof. Slavko Bernik
- 17. Irradiation and Analysis of Si Samples Asst. Prof. Saša Novak Krmpotič
- MODEF Creazione e Sperimentazione Congiunta di Modelli per l'Ottimizzazione dell'Utilizzo di Energia Fotovoltaica Dr. Zoran Samardžija

NEW CONTRACTS

- The Study of Self-cleaning and Abrasion Resisting Properties of Carbon-, Para-aramidor Glass-fibre-based Composite Materials by Applying Photocatalytic and/or Mechanical Resistant Nanoparticles Asst. Prof. Sašo Šturm
- 2. Multipole Magnetisation of NdFeB Bonded Magnets for Rotor Application
- Prof. Spomenka Kobe
 Cofinancing of the L2-4097 Application Project: High-coercivity Nd-Fe-B Bonded Magnets for Automotive Applications
- Prof. Spomenka Kobe
 Cofinancing of the L2-4192 Application Project: Materials and Technologies for Applications of ZnO-based Thick Film Varistors and Oxide Thermoelectrics Asst. Prof. Slavko Bernik
- Cofinancing the L2-4099 Application Project: Protected Permanent Magnets for Advanced High-Temperature Applications Asst. Prof. Paul John McGuiness

VISITORS FROM ABROAD

- Prof. Bojana Obradović, Prof. Vesna Misković-Stanković, Jovana Zvicer, Tehnološko-1. metalurški fakultet, Univerzitet u Beogradu, Belgrade, Serbia, 25. 1. 2013
- Prof. Hiroshige Kikura, Tokyo Institute of Technology, Tokyo, Japan, 25. 2. 2013 2 3. Dr. Meltem Sezen, Sabanci University, Nanotechnology Research and Application
- Center, Istanbul, Turkey, 17.-22. 3. 2013 Dr. Guorong Li, Chinese Academy of Science, Shanghaj, China, 3.-7. 4. 2013 4
- Samed Cetinkaya, Technology and R&D Application and Research Center, Mustafa 5. Kemal University, Hatay, Turkey, 4. 4.-31. 12. 2013
- 6. Xiangkai Xiao, Chinese Academy of Science, Shanghai Institute of Ceramics, Shanghai, China, 3. 4.-30. 9. 2013
- Prof. Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 20.-27. 2. 2013
- 8. Enrico Catalano, University of Piemonte Orientale "A. Avogadro", Laboratory of Biomedical and Dental Materials, Novara, Italy, 22. 4.-24. 5. 2013
- Dr. Branko Matović, Institut za nuklearne nauke Vinča, Beograd, Serbia, 28. 4.-4. 5. 2013 0 Dr. Jakub Michalski and Marta Bojarska, Wydział Inżynierii Materiałowej Politechniki 10.
- Warszawskiej, INMAT, Warszaw, Poland, 9. 5. 2013 11. Prof. Boštjan Markoli, Dr. Iztok Naglič, Faculty of Natural Sciences, University of Ljubljana, 9. 5. 2013
- Alessia Bolla, Politecnico di Torino, Torino, Italy, 25. 5.-28. 7. 2013
- 13. Dr. Cesar de Julian Fernandez, Dr. Claudio Sangregorio, Dr. Elisabetta Lottini, Dr. Alberto Lopez Ortega, Consorzio interuniversitario nazionale per la scienza e tecnologia dei materiali - INSTM, Florence, Italy, 30.-31. 5. 2013
- Dr. Alberto Bollero, María Jesús Villa, Dr. Julio Camarero, The Institute for Advanced Studies in Nanoscience - IMDEA, Madrid, Spain, 30.-31. 5. 2013
- Dr. Irena Škulj and Uroš Bavdek, Magneti d.d. Ljubljana, Ljubljana, Slovenia, 30.-31. 5. 2013 16. Judit Almunia, Dr. Ana Belen Seoane, Ingeniería magnética aplicada s.l. - IMA s.l., Barcelona, Spain, 30.-31. 5. 2013
- 17. Prof. José Francisco Fernández, Dr. Adrián Quesada, Agencia estatal consejo superior de investigaciones científicas - CSIC, Madrid, Spain, 30.-31. 5. 2013
- Dr. S. Erokhin, Dr. Dimitri Berkov, Verein zur förderung von innovation durch 18. forschung, entwicklung und technologietransfer e.v. - INNOVENT, Jena, Germany
- 19. Dr. Mogens Christensen, Aarhus universitet AU, Aarhus, Denmark, 30.-31. 5. 2013
- Dr. Matylda Guzik, Dr. Stefano Deledda, Institutt for energiteknikk IFE, Kjeller, Norway, 20.30.-31. 5. 2013

- 21. Dr. Bogi Bech Jensen, Muhammad Fasil, Danmarks Tekniske Universitet DTU, Kongens Lyngby, Denmark, 30.-31. 5. 2013
- 22. Dr. Pilar Marín, Ana Aragón, Universidad complutense de Madrid UCM, Madrid, Spain, 30.-31. 5. 2013
- 23. Prof. Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 5.-10. 5. 2013
- 24. Prof. Nazanin Emami, Arash Golchin, Fatima Nowshir, Silvia Suner, Stephan Schnabel, Alaleh Safari, Jorge Rituerto, Jinxia Li, Lule tekniska universitet, Lule , Śweden, 4. 6. 2013
- 25 Prof. Werner Mader, Institut für Anorganische Chemie - Univeristät Bonn, Bonn, Germany, 31. 7.-11. 8. 2013
- 26 Prof. Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 25.-28. 8. 2013
- 27 Dr. Claudia Silva, Faculdade de Engenharia da Universidade do Porto - FEUP, Porto, Portugal, 23.-27. 9. 2013
- 28 Dr. Adrian Silva, Faculdade de Engenharia da Universidade do Porto, Departemento de Engenharia Quimica, Porto, Potrugal, 20.-25. 8. 2013
- Dr. Mehmet Ali Gülgün, Dr. Cleva Ow-Yang, Sabanci University, Istanbul, Turkey, 29 18.-23.9.2013
- 30. Prof. Peter van Aken, Max-Planck-Institut Stuttgart, Stuttgart, Germany, 19.-20. 9. 2013 Prof. Joachim Kleebe, Dr. Marc Rubat du Merac, Technische Universität Darmstadt,
- Darmstadt, Germany, 9.-12. 10. 2013 Dr. Gerhard Niedermayr, Rudolf Hartmann, Naturhistorisches Museum Wien, Vienna Austria, 16.-17. 10. 2013
- Dr. Allan Walton, Dr. Vicky Mann, Magnetic Materials Group (MMG), Metallurgy and Materials, University of Birmingham, Birmingham, United Kingdom, 1.10.2013
- 34. Dr. Katarina Ćirić, Dr. Jana Radaković, Institut of Nuclear Sciences Vinča, Belgrade, Serbia, 12.-17. 11. 2013
- 35. Prof. Mihály Pósfai, Univesity of Veszprem, Veszprem, Hungary, 20. 11. 2013
- 36. Prof. Monica Ferraris, Politecnico di Torino, Torino, Italy, 15. 11. 2013

22. Ana Gantar, B. Sc.

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26. Rok Kocen, B. Sc.

25. Vanja Jordan, B. Sc.

27. Nina Kostevšek, B. Sc

28. Mateja Košir, B. Sc.

29. Matic Krivec, B. Sc.

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35. Rok Rudež, B. Sc.

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30. Alenka Lenart, B. Sc.

31. Martina Lorenzetti, B. Sc.

33. Matejka Podlogar, B. Sc.

36. Nadežda Stanković, B. Sc.

34. Mojca Presečnik, B. Sc.

23. Dr. Barbara Horvat, left 01.10.13

- Prof Jean-Marie Dubois, Institut Jean Lamour, Nancy, France, 5.-12. 10. 2013 37 Dr. Nikola Novaković, Dr. Jasmina Grbović Novaković, Dr. Ljiljana Matović, Sandra 38
- Kurko, Institut of Nuclear Sciences Vinča, Belgrade, Serbia, 29. 10.-4. 11. 2013 39. Prof. Jean-Marie Dubois, Dr. Vincent Fournee, Dr. Julien Ledieu, Dr. Emilie Gaudry, Dr. Merie-Cecile De Weerd, Dr. Pascal Boulet, Institut Jean Lamour, Nancy, France, 5.-13.12.2013

STAFF

Researchers

- Asst. Prof. Slavko Bernik 1
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- Asst. Prof. Nina Daneu 3.
- Asst. Prof. Goran Dražić* 4.
- 5 Prof. Spomenka Kobe, Head
- Asst. Prof. Matej Andrej Komelj 6.
- Asst. Prof. Paul John Mcguiness
- Asst. Prof. Saša Novak Krmpotič 8
- Asst. Prof. Aleksander Rečnik 0
- 10 Dr Zoran Samardžija
- 11. Asst. Prof. Sašo Šturm
- 12. Asst. Prof. Kristina Žužek Rožman

Postdoctoral associates

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- 14. Dr. Aljaž Iveković
- 15. Dr. Andraž Kocjan
- 16. Dr. Benjamin Podmiljšak
- 17. Dr. Marko Soderžnik

18. Dr. Kristina Žagar

Postgraduates

- 19. Anže Abram, B. Sc. 20. Muhammad Shahid Arshad, B. Sc.
- 21. Sandra Drev, B. Sc.

BIBLIOGRAPHY

- **ORIGINAL ARTICLE**
 - 1. Marcela Achimovičová, Nina Daneu, A. Zorkovská, Martin Fabián, "The use of de-aggregating agents in ZnSe mechanochemical synthesis", J. mater. sci., Mater. electron., vol. 24, no. 10, pp. 3686-3693, 2013.
- 2. Bojan Ambrožič, Sašo Šturm, Miha Jeršek, Breda Mirtič, "Structure of the chondrules and the chemical composition of olivine in meteorite Jesenice", Geologija, knj. 56, no. 1, pp. 19-28, 2013.
- 3. Sigrid Bernstorff, Václav Holý, Jan Endres, Václav Valeš, Jaroslav Sobota, Zdravko Siketić, Iva Bogdanović-Radović, Maja Buljan, Goran Dražić, "Co nanocrystals in amorphous multilayers - a structure study", J. Appl. Crystallogr., vol. 46, no. 6, pp. 1711-1721, Dec. 2013.

- 5. Maja Buljan et al. (13 authors), "Ge quantum dot lattices in Al_2O_3
- multilayers", *J. nanopart. res.*, vol. 15, no. 3, pp. 1485-1-1484-13, 2013. 6. Maja Buljan *et al.* (11 authors), "Tuning the growth properties of Ge quantum dot lattices in amorphous oxides by matrix type", J. Appl. Crystallogr., vol. 46, no. 5, pp. 1490-1500, 2013.
- 7. Maja Buljan, Nikola Radić, Iva Bogdanović-Radović, Zdravko Siketić, K. Salamon, M. Jerčinović, Mile Ivanda, Goran Dražić, Sigrid Bernstorff, "Influence of annealing conditions on the structural and photoluminescence properties of Ge quantum dot lattices in a continuous Ge + Al_2O_3 film", *Phys. status solidi, A Appl. mater. sci.*, vol. 210, issue 8, pp. 1516-1521, 2013.
- 8. Jovana Ćirković, Katarina Vojisavljević, Maja Šćepanović, Aleksander Rečnik, Goran Branković, Zorica Branković, Tatjana Srećković, "Hydrothermally assisted complex polymerization method for barium strontium titanate powder synthesis", J. sol-gel sci. technol., vol. 65, issue 2, pp. 121-129, 2013.
- 9. Nina Daneu, Nives Novak Gramc, Aleksander Rečnik, Marieta Maček, Slavko Bernik, "Shock-sintering of low-voltage ZnO-based varistor ceramics with Bi4Ti3O12 additions", J. Eur. Ceram. Soc., vol. 33, issue 2, pp. 335-344, 2013.
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- 11. Sandra Drev, Aleksander Rečnik, Nina Daneu, "Twinning and epitaxial growth of taaffeite-type modulated structures in BeO-doped MgAl₂O₄", CrystEngComm (Camb., Online), vol. 15, issue 14, pp. 2640-2647, 2013.
- 12. Andreja Gajović, Jelena Vukajllović Pleština, Kristina Žagar, Milivoj Plodinec, Sašo Šturm, Miran Čeh, "Temperature-dependent Raman spectroscopy of BaTiO₃ nanorods synthesized by using a templateassisted solgel procedure", J. Raman spectrosc., vol. 44, no. 3, pp. 412-420.2013.
- 13. Davor Gracin, Zdravko Siketić, Krunoslav Juraić, Miran Čeh, "Analysis of amorphous-nanocrystalline silicon thin films by time-of-flight elastic recoil detection analysis and high-resolution electron microscopy", In: Proceedings of the NANOSMAT, 7th International Conference on Surfaces, Coatings and Nanostructured Materials, 18-21 September 2012, Prague, Czech Republic, Appl. Surf. Sci., vol. 275, pp. 19-22, 2013.
- 14. Anton Gradišek, Dorthe Ravnsbæk, Stanislav Vrtnik, Andraž Kocjan, Janez Lužnik, Tomaž Apih, Torben R. Jensen, Alexander V. Skripov, Janez Dolinšek, "NMR study of molecular dynamics in complex metal borohydride $LiZn_2(BH_4)_5$ ", *The journal of physical chemistry. C*, Nanomaterials and interfaces, vol. 117, no. 41, pp. 21139-21147, 2013.
- 15. Nejc Hodnik, Milena Zorko, Barbara Jozinović, Marjan Bele, Goran "Severe accelerated Dražić, Stanko Hočevar, Miran Gaberšček, degradation of PEMFC platinum catalyst: a thin film IL-SEM study", Electrochem. commun., vol. 30, pp. 75-78, 2013.
- 16. Aljaž Iveković, Saša Novak, Goran Dražić, Darina Blagoeva, Sehila Gonzalez de Vicente, "Current status and prospects of SiC_f/SiC for fusion structural applications", J. Eur. Ceram. Soc., vol. 33, no. 10, pp. 1577-1589, 2013.
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- 22. Zorica Lazarević, Čedomir Jovalekić, A. Milutinović, Dušan Sekulić, Valentin Ivanovski, Aleksander Rečnik, Božidar Cekić, Nebojša

Romčević, "Nanodimensional spinel $NiFe_2O_4$ and $ZnFe_2O_4$ ferrites prepared by soft mechanochemical synthesis", In: Proceedings of the International Symposium on Applications of Ferroelectrics: European Conference on the Applications of Polar Dielectrics; International Symposium Piezoresponse Force Microscopy and Nanoscale Phenomena in Polar Materials, 9-13 of July, 2012, Aveiro, Portugal, J. Appl. Phys., vol. 113, no. 18, pp. 187221-1-187221-11, 2013.

- 23. Zorica Lazarević, Čedomir Jovalekić, Aleksander Rečnik, Valentin Ivanovski, Aleksandra Milutinović Živin, Maja J. Romčević, Miodrag B. Pavlović, Božidar Cekić, Nebojša Romčević, "Preparation and characterization of spinel nickel ferrite obtained by the soft mechanochemically assisted synthesis", Mater. res. bull., vol. 48, issue 2, pp. 404-415. 2013.
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MENTORING

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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 for use in the microwave frequency range, and fluorescent materials.

In 2013 our investigations have focused on several important materials, i.e., materials containing magnetic nanoparticles, multifunctional nanocomposites, fluorescent materials, and ferroelectric, semiconducting materials for the preparation of thermistors.

The research on magnetic nanoparticles has mainly looked at magnetic carriers for applications in magnetic separation in biotechnology, in environmental technologies, and in medicine. The magnetic separation is based on the selective bonding of targeted species, i.e., ions, molecules, cells, or microorganisms, onto the magnetic carriers followed with their separation from the mixture using an external magnetic field. Simple magnetic iron oxide is Head: used as the material for the magnetic carriers, which have to be composed of magnetic nanoparticles that are small Prof. Darko Makovec enough to be in the superparamagnetic state, i.e., below approximately 15 nm. Individual superparamagnetic nanoparticles are usually not efficient in magnetic separation, because of a too small magnetic force acting on them in a magnetic-field gradient, which is the result of their very small volume. In order to improve the ability of magnetic separation, the superparamagnetic nanoparticles have to be agglomerated into nanoclusters, optimally with size

from 50 to 100 nm. The superparamagnetic nanoclusters were synthesized using the hetero-agglomeration (self-assembly) of the nanoparticles in the suspensions of superparamagnetic iron-oxide maghemite nanoparticles applying an attractive electrostatic force between nanoparticles with an opposite surface charge or the chemical reactions between surface molecules. For the synthesis of the nanoclusters, the maghemite nanoparticles were coated with a thin layer of silica and grafted by silane molecules with either terminal amino groups (for a positive surface charge in aqueous suspensions), or with terminal carboxyl groups (a negative surface charge). For an easier analysis, one type of the

nanoparticles was changed with equally functionalized silica nanoparticles (Figure 1). The hetero-agglomeration of the two types of nanoparticles caused by the electrostatic interactions or by the chemical reactions between the surface amino groups and activated carboxyl groups has been systematically studied. The hetero-agglomeration using

the chemical interactions between the nanoparticles resulting from direct reactions between the amino and carboxyl groups of the molecules at their surfaces appeared to be more efficient compared to hetero-agglomeration using electrostatic interactions. The kinetics of the hetero-agglomerates' formation in the suspension has been studied in cooperation with the Department for Complex Matter (F7).

Novel superparamagnetic nanoclusters with a size of approximately 60 nm were synthesized using the chemically-driven crosslinking of functionalized superparamagnetic nanoparticles. Their surface was then coated with a thin silica shell. The fluorescent molecules were incorporated into the silica shell for tracking of the nanoclusters with methods based on fluorescence microscopy. Special attention has been given to an adaptation

of the nanoclusters' surface properties to the demands of specific applications. The nanoclusters' surface needs to be suitably functionalized with specific functional groups that enable further (bio)conjugations. The nanoclusters were functionalized either with organosilane molecules, which form covalent bonds with the silica shell, or using the layer-by-layer deposition of cationic and anionic polyelectrolytes. Nanoclusters functionalized with different molecules were investigated in the magnetic separation of heavy-metal ions from contaminated water. Magnetic nanoclusters could also be interesting in many other applications where a relatively large magnetic force acting on the nanocluster in a magnetic field gradient could be beneficially exploited. Magnetic drug delivery and cell-transfection (magnetofection) using magnetic nanoclusters are the most promising applications in the biomedical field.

The hetero-agglomeration of nanoparticles in their aqueous suspensions is based on electrostatic interactions between the nanoparticles displaying an opposite surface charge or based on chemical reactions between molecules on their surfaces.

Figure 1: TEM image (left) and SEM image (right) of nanoclusters synthesized using the heteroagglomeration of iron-oxide maghemite nanoparticles and silica nanoparticles in the suspension.





K-8

We have also continued our research on magnetic nanoparticles for cancer treatment by magnetic hyperthermia. Magnetic hyperthermia is based on the heating ability of magnetic nanoparticles, localized in tumour tissue, when exposed to alternating magnetic fields. Depending on the magnetic properties of the magnetic nanoparticles the heating can be a consequence of the lag between the magnetization and the AC field (for superparamagnetic nanoparticles) or of the hysteresis losses (for ferrimagnetic nanoparticles). The magnetic iron oxide nanoparticles

Magnetic coupling in composite nanoparticles composed of a hard-magnetic hexaferrite core and a soft-magnetic maghemite shell has been analysed. The coupling results in an increase of the energy product $|BH|_{max}$ by more than 50 % compared to the $|BH|_{max}$ of the core nanoparticles. are believed to be the most suitable magnetic nanoparticles for biomedical applications, because their use has been approved by the American Food and Drug Administration (FDA). In collaboration with the Powder Technology Laboratory, EPFL Switzerland we have developed a synthesis method that enables good control over the size of the nanoparticles. The nanoparticles were synthesized by a hydrothermal process in the presence of ricinoleic acid, which acts as a surfactant. The surfactant bonds to the nanoparticle surfaces and inhibits their growth. The influence of the synthesis temperature and the concentration of ricinoleic acid on the nanoparticle average size have been systematically studied. The nanoparticle average size was successfully

controlled at values ranging between 9 nm and 30 nm. While the nanoparticles smaller than ~14 nm exhibited superparamagnetic behaviour the larger nanoparticles demonstrated ferromagnetic behaviour. In collaboration with the School of Pharmaceuticals Sciences, University of Genève-University of Lausanne, Switzerland, we have studied the heating properties of the nanoparticles. The measurements showed that the optimal heating characteristics were exhibited by the ferrimagnetic nanoparticles. Additionally, the nanocomposites that contained the magnetic nanoparticles in a polymer matrix were prepared. Such nanocomposites are suitable for the fixation of vertebrae affected by cancer and enable additional treatment with magnetically induced hyperthermia.

A part of our research was also devoted to magnetic nanoparticles with an adaptable Curie temperature (T_c) for use in self-regulating magnetic hyperthermia. The T_c limits the temperature to which the nanoparticles are being heated in an external magnetic field, and thus an external temperature control is not required. In cooperation with the Faculty of Chemistry and Chemical Technology, University of Maribor, we have studied the synthesis and properties of the nanoparticles made of those magnetic materials, where the T_c can be tuned to the therapeutic values by adapting their composition. The main focus was on spinel ferrite Mg(Ti)Fe₂O₄ and on different alloys from the systems Cu-Ni and Cr-Ni.

The synthesis of cobalt-ferrite nanoparticles ($CoFe_2O_4$) and their stable suspensions was also investigated. We focused on spinel ferrite nanoparticles in the size region from sizes where superparamagnetism dominates to the region where ferrimagnetism dominates the magnetic properties. For certain applications, colloidal suspensions



Figure 2: Magneto-electric composite synthesized by the assembly of $CoFe_2O_4$ nanoparticles and $Pb(Zr,Ti)O_3$

of ferrimagnetic nanoparticles in various carrier liquids are desired. The preparation of the suspensions and their colloidal and magnetic properties have been systematically studied. Ricinoleic acid was used as the surfactant for the nonpolar media and citric acid for the aqueous media. The CoFe₂O nanoparticles were synthesized by the co-precipitation of Fe³⁺/Co²⁺ ions from the aqueous solution. The addition of a strong base to an aqueous solution of cations results in the precipitation of an amorphous Co-deficient phase and Co(OH)₂. The precipitates react to form very small CoFe₂O₄ nanoparticles, which at a later stage grow through the Ostwald ripening process, reaching a final size of ~14 nm. The synthesized nanoparticles displayed relatively high values of saturation magnetization and coercivity. The adsorption of the citrate anion on the nanoparticle surfaces enabled the preparation of the aqueous colloidal suspensions. The adsorption of ricinoleic acid on the nanoparticle surfaces enabled the preparation of a colloidal suspension in toluene. However, the ricinoleic acid was not efficient in preventing the agglomeration of nanoparticles larger than ~15 nm in toluene. The markedly

different colloidal behaviour was qualitatively described by the total interaction energy between the two nanoparticles. The citrate-anion-adsorbed nanoparticles in the aqueous media are negatively charged and therefore repulsive. The interaction between the ricinoleic-acid-adsorbed nanoparticles is attractive. The attraction in toluene is larger than the thermal energy for nanoparticles larger than ~15 nm. Both suspensions displayed superparamagnetic behaviour, despite the ferrimagnetic nature of the dispersed nanoparticles.

We also cooperated in nanotoxicology research with the Biotechnical Faculty, University of Ljubljana, where we provided our expertise in the synthesis, functionalization and characterization of nanoparticles.

 $CoFe_2O_4$ shows magnetic properties that are not typical for spinel ferrites, i.e., a high magnetic anisotropy, which results in high coercivity and magnetostriction. It shows the largest magnetostriction among oxide materials and

is therefore suitable for applications in multifunctional composites like: magneto-electrics, in which magnetic and ferroelectric properties are mechanically coupled. The properties of such composites depend on the basic properties of the constituent phases and on the specific phase distribution in the material. We prepared columnar structures with a magnetically directed assembly of CoFe_2O_4 nanoparticles from the suspensions. The effect of the colloidal properties on the morphology of the columns has been systematically studied. The results showed that the density

distribution of the columns on a substrate, their height and roughness depend on the nanoparticle concentration in the suspension, the wetting angle and the evaporation rate of the solvent. Thus, various 3D structures can be assembled from the $CoFe_2O_4$ nanoparticles by tuning the magnetic field distribution using a template. The anisotropic $CoFe_2O_4$ 3D structures can be used as a basis for magneto-electric composites with a 1-3-type

We showed a significant inverse magnetoelectric effect in $CoFe_2O_4/Pb(Zr,Ti)O_3$ ceramic composites.

structure. Their preparation using the electrophoretic deposition of $Pb(Zr,Ti)O_3$ on top of the $CoFe_2O_4$ columns has been studied in cooperation with Electronic Ceramics Department (K5) (Figure 2). We also prepared $CoFe_2O_4$ / $Pb(Zr,Ti)O_3$ composite ceramics by co-sintering of the constituent powders at 950°C. The magnetic properties of these ceramics composites were greatly affected by an electric field.

A large part of our research was devoted to the synthesis and detailed characterisation of composite nanoparticles synthesized using a coating of thin shells of magnetic iron oxide onto different core nanoparticles using simple precipitation from aqueous solutions. By coating a shell of soft-magnetic spinel iron oxide maghemite $(g-Fe_2O_3)$ onto hard-magnetic barium-hexaferrite $(BaFe_{12}O_{19})$ platelet cores the "sandwich"-type composite nanoparticles were synthesized. Such sandwich nanoparticles are composed of the hexaferrite core in between the two spinel layers. The spinel layers grow epitaxially on the hexaferrite core with spinel {111} planes parallel to the hexaferrite basal {0001} planes. Magnetic coupling between the two components has been analysed. The magnetic coupling results in a large increase in the energy product $|BH|_{max}$ by more than 50 % compared to the $|BH|_{max}$ of the core nanoparticles. When the ultrafine hexaferrite core nanoparticles, with a size below 10 nm, were coated the two components chemically reacted. The homogeneous product nanoparticles are formed as the result of the chemical reaction. The product nanoparticles differ in composition and in structure from any known compound in the BaO-FeO_x system. The temperature stability of the product nanoparticles has been studied using high-resolution electron microscopy (HREM) and magnetic measurements.

The magnetic shell was also coated onto the core nanoparticles of other functional materials including photocatalytic anatase nanoparticles (TiO_2). On the other hand, the possibility of coating shells made of other magnetic spinels, especially of hard-magnetic cobalt ferrite, has been investigated.

We continued our research on the synthesis of nanocomposite particles used for the decomposition of organic pollutants in water. The nanocomposite particles are composed of photocatalytic anatase (TiO_2) nanoparticles coated onto agglomerates of superparamagnetic maghemite (Fe₂O₃) nanoparticles. For the photocatalytic purification, the particles are dispersed in polluted water. The surface anatase layer provides a high photocatalytic activity, while the superparamagnetic cores enable the separation of the particles from the suspension after the purification and

their re-use. The research was mainly oriented to mechanisms enabling an increase in the photocatalytic activity of the materials applying electronic interactions at the interface between the two semiconducting components, the anatase (band gap pasu $\rm E_g \sim 3.2~eV)$ and the maghemite ($\rm E_g \sim 2.3~eV)$). It appeared that the photocatalytic activity of the anatase nanoparticles is significantly increased when they are in contact with the maghemite nanoparticles. The photocatalytic activity of the anatase with aliovalent dopants, such as Fe³⁺ and W⁶⁺.

The studies in the field of magnetic materials for telecommunications were focused on the development of ceramic films for micro- and mm-wave applications. We broadened our research on the preparation of magnetically oriented BaFe₁₂O₁₉ thick films in a magnetic field on the comparative study of the effect of the shape anisotropy versus magnetic interparticle interaction. We were able to achieve a magnetic orientation higher than 80% only by the deposition of the BaFe₁₂O₁₉ nanoplates on a substrate without any external field. This kind of assembly during the drying of the suspensions was attributed to the magnetic interparticle interaction. Such films are suitable for self-biased magnetic devices, including nonreciprocal microwave devices.

The studies in hexaferrite materials were also focused on the hydrothermal and coprecipitation synthesis of $BaFe_{12}O_{10}$ nanoplates and the effect of the



Figure 3: An in-plane magnetic hysteresis of the composite nanoparticles (NC) composed of a hard-magnetic hexaferrite core in between the two soft-magnetic spinel layers is compared with the hysteresis of hexaferrite core nanoparticles (HF) and the hysteresis of a mixture of hexaferrite and spinel (S) nanoparticles. The comparison suggests magnetic coupling between the components in the composite.

chemical substitution of Fe³⁺ with Sc³⁺ on the size of the nanoplates. The size distribution can be effectively narrowed with the Sc³⁺ regardless of the synthesis conditions. At the same time, the magnetic properties of the nanoplates are improved significantly. Magnetic liquid crystals were developed from these nanoplates in cooperation with the Department of Condensed Matter (F7). The Sc-based nanoplates were also incorporated into a polymer matrix and

We showed that nanoplates with applicable magnetic properties can be synthesized by a partial chemical substitution of Fe³⁺ with Sc³⁺ in BaFe₁₂O₁₉ and that these nanoplates are suitable for the preparation of new magnetooptic materials: magnetic liquid crystals and transparent magnetic polymer composites. we prepared a transparent magnetic polymer composite in cooperation with the Faculty of Chemistry and Chemical Technology of University of Maribor. Both types of new composites exhibit applicable magneto-optic properties.

We have started with a study of fluorescent optical materials. We studied the synthesis of fluoride nanoparticles doped with lanthanides and their nanocomposites with a silica shell. The main focus was oriented toward the control of the particle size, the suspension stability and the chemical stability of fluorides in an aqueous environment. The specified particle size is required for the incorporation of the nanoparticles into the optical-fibre

technology. These studies are conducted in the frame of a common project with a company Optacore: "Optical fibres doped with fluorescent nanoparticles". Fluorescent fluoride nanoparticles were suggested as alternative bio-markers. They have to show a chemical stability in aqueous environment and they are to be used in bio-medicine. However, we showed that the fluoride nanoparticles were not stable in water suspensions and they require special care before their application in bio-medicine.

The research in the field of semiconducting ceramics has been focused on the effect of the positive temperature coefficient of resistivity (PTCR). A BaTiO₃-based composite composed of undoped semiconducting BaTiO₃ grains and highly resistive BaTiO₃ grains was prepared. We showed that such a composite, which mimic a conventional BaTiO₃ thermistor, exhibits a significant anomaly in electrical resistivity due to the disconnection of the network of semiconducting BaTiO₃ grains at the Curie temperature. The anomaly in resistivity was of three orders of magnitude. The result of this investigation will change the basic picture of the functioning of this ceramic, which is in its mature age of exploitation.

In the field of high-temperature thermistors (PTC resistors) we continued to investigate the processes of their formation in ferroelectric ceramics from the systems $BaTiO_3 - Na_{0.5}Bi_{0.5}TiO_3$. The PTC resistors displaying a Curie temperature of 180 °C and low room-temperature resistivity were developed. Unlike the conventional high-temperature PTCR materials available on the market the developed material contains no poisonous lead.

Some outstanding publications in the past year

- Kralj, S., Rojnik, M., Romih, R., Jagodič, M., Kos, J., Makovec, D.: Effect of surface charge on the cellular uptake of fluorescent magnetic nanoparticles. *J. nanopart. res.*, 2012, vol. 14, no. 10, 1151-1–1151-14
- Mertelj, A., Lisjak, D., Drofenik, M., Čopič, M.: Ferromagnetism in suspensions of magnetic platelets in liquid crystal. *Nature*, ISSN 0028-0836, 2013, vol. 504, no. 7479, 237–241

INTERNATIONAL PROJECT

 COST IC1208; Integrating Devices and Materials: A Challenge for New Instrumentation in ICT COST Office Prof. Darko Makovec

RESEARCH PROGRAM

1. Advanced Inorganic Magnetic and Semiconducting Materials Prof. Darko Makovec

NEW CONTRACTS

- 1. Optical Fibers Doped with Fluorescent Nanoparticles Optacore, d. o. o. Asst. Prof. Darja Lisjak
- Research and Development of PTCR-effect Semiconducting Ceramics without Environmentally Harmful Lead Oxide Stelem, d. o. o., Žužemberk Dr. Igor Zaic
- Development of Analytical Methods and Characterisation of Pharmaceutical Form Containing Iron-Oxide Nanoparticles Lek, d. d.

Prof. Darko Makovec

VISITORS FROM ABROAD

- 1. Dr. Marin Tadič, Vinca Institute, Condensed Matter Physics Laboratory, University of Belgrade, Beograd, Serbia, 6. 8.–30. 10. 2013
- Bernardo Maestro Maria Beatriz, Instituto de Cermica y Vidrio (CSIC), Madrid, Spain, 4. 11.–4. 12. 2013
- 3. Dr. Lionel Maurizi, LTP EPFL, Switzerland, 1.-7. 12. 2013
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PUBLISHED CONFERENCE CONTRIBUTION

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DEPARTMENT FOR ADVANCED **MATERIALS**

K-9

The main activities of the department encompass basic and applied research within the fields of energy materials, biomaterials and electronic materials. Among the important objectives are the development of new, efficient oxides for high-temperature thermoelectric energy conversion, materials with improved antibacterial and photocatalytic effects and the development of thin films and nanostructured powders of functional oxides for various electronic applications.

Thermoelectric oxides

Continued research on thermoelectric layered cobaltates Ca. Na Co O showed that intergrown structures exhibit a Seebeck coefficient higher than both the end members, Na CoO₂ and Ca₂Co₄O₆. With an increase in x the electrical conductivity can be tailored from semiconducting to metallic behaviour, which enables control of the power factor of the material. The highest measured power factor was at compositions with $x \sim 1$, which also exhibit environmental stability as opposed to pure Na_xCoO_y. In the scope of the industrial project with Epcos, a part Head: of TDK-EPC company, we performed a study of the development of intergrown structures and their influence on the **Prof. Danilo Suvorov** texturing and, consequently, the electrical conductivity. We found that the formation of an intergrown structure prior to the sintering stage crucially influences the microstructure and, consequently, the electrical conductivity. We have also found that intergrown structures are stable in an air atmosphere up to 930°C, above which a reversible loss of oxygen takes place, resulting in the formation of a secondary phase CoO. In an inert atmosphere the reversible decomposition takes place already at temperatures below 500°C. The findings indicate that based on coherently intergrown structures Ca_{2,y}Na_yCo₄O₉ high-temperature p-type thermoelectric materials with an operating range up to ~900°C can be synthesized. At 700°C ceramics with the nominal composition Ca, Na, Co, O, exhibit a figure of merit zT~0.3. The results obtained so far also indicate that a further improvement of the conversion efficiency is possible by reducing thermal conductivity and so controlling the atmosphere during processing and thus influencing the formation of nano-inclusions within the coherently intergrown matrix.

Antibacterial and photocatalytic materials

Nanocomposite materials based on TiO, and Pt particles were prepared via two syntheses, i.e., hydrothermal synthesis and sonochemical synthesis, followed by thermal treatment in a reducing atmosphere at 400°C for 3 h. The hydrothermally synthesized TiO₂/Pt consisted of TiO₂ (average particles size 16 nm) in the anatase and the rutile crystal modification. TiO₃/Pt prepared by the sonochemical synthesis crystallized as the TiO₂ (average particle size 9 nm) anatase and brookite. The hydrothermal synthesis enabled the formation of two types of Pt particles: the Pt particles (12-17 nm) that were attached on the TiO, surface and the Pt particles that existed as an isolated phase (up to 45 nm). In the case of the sonochemical synthesis the Pt particles (up to 5 nm) formed a composite with the TiO, particles. The XPS surface analysis of the prepared TiO,/Pt revealed that the formed Pt existed as Pt⁰ and Pt²⁺. The presence of the free hydroxyl groups was identified utilizing the FTIR spectroscopy. The free surface hydroxyl groups were detected only in the case of the hydrothermally synthesized TiO₄/Pt. The photocatalytic activity was



Figure 1: Hydrothermally synthesized TiO,/Pt.



Figure 2: Sonochemical synthesized TiO,/Pt.





Figure 3: SEM image of BSO thin films deposited on Si/SiO_TO_P substrate annealed at 700°C/1h.



Figure 4: The degradation rate of the RhB solution under UV irradiation with the photocatalyst BSO film and P25 film

determined by monitoring the degradation of the aqueous solution of the azo dye methylene blue under UV and Vis irradiation. The measurements revealed that the UV photocatalytic activity of the hydrothermally synthesized TiO_2/Pt was 16-times higher than the activity of the sonochemically synthesized TiO_2/Pt . Under Vis irradiation the photocatalytic performance of the hydrothermally synthesized TiO_2/Pt exceeded the activity of the sonochemically prepared TiO_2/Pt by 5-times. The higher photocatalytic efficiency of the hydrothermally synthesized TiO_2/Pt was ascribed to the presence of the free surface hydroxyl groups. Such hydroxyl groups form with the photogenerated holes from the TiO_2 valence band strong hydroxyl radicals, which degraded the organic compounds adsorbed on the surface of the TiO_2 .

Photocatalytic films based on the sillenite compound $Bi_{12}SiO_{20}$ (BSO) were prepared using the polymerizable complex method. The obtained BSO films had a porous microstructure with an average size of the grains equal to 1µm. Its photocatalytic activity was evaluated with the degradation of the aqueous organic pollutant Rhodamine B under UV-light irradiation. The $Bi_{12}SiO_{20}$ films showed comparable photocatalytic performance in the degradation of the RhB solution under UV-light irradiation as the reference Degussa P25 film. Namely, both photocatalytic films BSO and P25 degraded over 82% of the RhB solution within the irritation time of 150 min.

In 2013 we also focused on the syntheses of new antibacterial materials that include a gallium component. This should increase the efficiency of the functionalized gold nanoparticles on hydroxyapatite, which have recently been developed at this department, but avoid the increase of their harmfulness towards eukaryotic (human) cells. Using a sonochemical method we successfully prepared nanocomposites of gold nanoparticles, functionalized with amino acids, and hydroxyapatite with Ga(III) ions, most probably in its interstitials. All the nanoparticles in the composite are spherical, of very similar size (with a diameter of approx. 5 nm with histidine, approx. 10 nm with arginine and approx. 20 nm with glycine) and well separated on the hydroxyapatite nanorods. We also managed to obtain a composite of hydroxyapatite with spherical gallium nanoparticles, covered with GaOOH. A gold nanoshell with different amino acids attached is being added to these nanoparticles, in order to obtain functionalized core-shell nanodevices for targeted drug delivery of an antibacterial (gallium) core.



Figure 5: Nanocomposite of arginine-functionalized Au nanoparticles and Ga(III)-containing hydroxyapatite under a transmission electron microscope.



Figure 6: TEM picture of histidine-functionalized Au nanoparticles on hydroxyapatite nanorods with incorporated Ga(III) ions

Functional oxides for electronic applications

In the field of the investigation of phase relations in ternary oxide systems where new compounds and/or solid solutions are stable and exhibit pronounced electric properties, we determined phase relations in the ternary systems La_2O_3 -TiO_2-CaO at 1400°C in previous research. This year we continued with investigations and we determined the crystallographic structure of the solid solution CaTiO_3-Ca_3La_4Ti_3O_{15}, which is stable along the whole tie line. We described a transition from one crystal structure into another and determined the microstructural and dielectric properties of these ceramics. For the synthesis of the single-phase ceramics a modified Pechini method was used.

We have also investigated ceramics based on the compound $CaCu_3Ti_4O_{12}$, which exhibit interesting dielectric properties and ceramics based on the solid solution $CaCu_3Ti_4O_{12}$. $CaCu_3Ru_4O_{12}$.

The research of BaTiO₂ particle formation was focused on (i) the topotactic transformation of various titanate precursors into BaTiO₂, (ii) the characterization of tetragonal BaTiO₂ particles, prepared under moderate hydrothermal conditions, (iii) the sintering of variously shaped BaTiO₃ particles and a determination of the dielectric properties. The aim of the first part was to explore possibilities for the preparation of defined shaped BaTiO₂ particles by preserving the shape of the titanate precursor. This kind of transformation is possible in liquid phase (hydrothermal and molten salt synthesis) under conditions that favour the epitaxial growth of BaTiO₂ on a titanate precursor. These conditions include a low lattice mismatch and a low density of surface defects. The comparison of the BaTiO₂ lattice parameters with those of the titanate precursors (Na₂Ti₂O₂ (NT) belts, K₂Ti₆O₁₃(KT) wires, K₁₃₃Li₁₃₃Ti₃₃₃O₈(KLT) plates) showed a mismatch greater than 4%. Epitaxial growth could occur, when the high strains are relieved by the formation of dislocations and grain boundaries. Our investigations revealed that the topochemical transformation of the titanate precursor into BaTiO₂ was better approached by the NT belts than by the KLT plates and KT wires. The morphology of the BaTiO₃ particles formed from the last precursor at low temperature (80-100°C) was found to be very similar to that obtained with the NT belts. The differences appeared at T≥150°C, where BaTiO, with a considerably higher degree of tetragonality was formed from KT compared to that from the other precursors. Raman spectroscopy, which gave information about the local structure, showed that the asymmetry within $[TiO_6]$ the octahedra was present already in BaTiO3, prepared at 100°C. According to the result of this technique, BaTiO₂ with a high degree of tetragonality formed from KT at 150≤T≤240°C. The differences in tetragonality for BaTiO, formed at different high-temperature ($150 \le T \le 240^{\circ}$ C) conditions could be better detected by XRD and DSC, because they gave information about long-range order. In XRD pattern, the tetragonality is evident from the splitting of the (200) diffraction line, while DSC gave the enthalpy of tetragonal to cubic phase transition. We found that tetragonality increased with an increase of the temperature and synthesis time. When the NaOH content exceeded the concentration needed for BaTiO₂ formation, the tetragonality decreased with an increase of the NaOH content.

The sintering studies of variously shaped (star- and square-like) cubic BaTiO₃ particles revealed that particle shape had an important influence on the grain growth and phase transformation. The sintering of square-like particles led to tetragonal ferroelectric and coarse grained (2-10 μ m) BaTiO₃ ceramics, while star-like particles preserved the cubic crystal structure without a significant increase in the grain size (1 μ m). High relative densities of 98% were achieved by two-step sintering, which is regarded as a promising method for controlling the grain growth. Based on this fact we assume that dielectric, ferroelectric and piezoelectric properties of BaTiO₃ ceramics could be tailored by the selection of the particle shape and the proper sintering conditions.

We have investigated the synthesis of Ag(Nb_xTa_{1,x})O₃ (x = 0.2-1) ceramics by a solid-state reaction method. Pure-phase ceramics with a relative density higher than 96% can be obtained, except for x = 0.2. As x decreases from 1, the dielectric constant at 2.9-4.4 GHz first increases from 222, reaches the maximum value of 491 for x = 0.65, and then decreases to 206 for x = 0.2. While the Q×f value increases monotonically from 72 GHz for x = 1 to 1.550 GHz for x = 0.2, although the ceramic with x = 0.2 is relatively porous and not single phase. The Ag(Nb_xTa_{1,x})O₃ (x = 0.5-1) ceramics show interesting tunable dielectric properties. When x = 1, unique "W"-shaped depend-

ences of dielectric constant and dielectric loss on DC bias are observed, indicating the coexistence of ferroelectricity and anti-ferroelectricity. Similar results are observed for x = 0.8 and 0.65, while only anti-ferroelectricity is indicated for x = 0.5. The anti-ferroelectricity can be observed based on a tunability measurement with the maximum DC of 125 kV/cm or even lower. However, much higher electric field of 175 kV/cm is needed for observing an anti-ferroelectric-like hysteresis loop. It is indicated that the tunability measurement is a more sensitive tool than the hysteresis loop for determining the anti-ferroelectricity.

 $Ag(Nb_{0.5}Ta_{0.5})O_3$ thin films have also been deposited on (0001) Al_2O_3 single-crystal substrates by pulsed laser deposition with a fluence of 1.5 J/ cm² and an oxygen pressure of 0.1 mbar, and they are characterized by XRD and RHEED. When the target-to-substrate distance is 55 mm, the repetition rate is 5Hz and the deposition time is 1 hour, polycrystalline $Ag(Nb_{0.5}Ta_{0.5})O_3$ primary phase is indicated from XRD for the deposition temperatures of 550-625°C. However, a small concentration of secondary phase can also be



Figure 7: Tunable dielectric properties for $Ag(Nb_xTa_{1x})$ $O_3(x=0.5-1)$ ceramics with "W"-shaped dependences of dielectric constant and dielectric loss on DC bias, indicating the coexistence of ferroelectricity and anti-ferroelectricity.



Figure 8: Plume created during laser ablation of $Ag(Nb_{0.5}Ta_{0.5})O_3$ ceramic target at 1.5 J/cm² laser energy and 0.1 mbar oxygen partial pressure in pulsed laser deposition system.



Figure 9: Cross-sectional view of the test resonators (a) and DC bias dependences of permittivity (ε (V)) and relative tunability of permittivity ($T\varepsilon$ (V)), measured at 3 GHz, of a test structure with the 440-nm-thick PMN-PT film (b).



Figure 10: Microstructural development of PMN-PT thin films pyrolysed at temperature a) 200°C, b) 300°C in c) 430°C and annealed at 650°C/20 min.

In the scope of the Center of Excellence in Nanoscience and Nanotechnology we installed the Empyrean X-ray diffractometer at the Advanced Materials Department, which is utilized mainly for the detailed structural characterization of single-crystal thin films. The delivered system enables the study of the epitaxial layers in terms of reciprocal spacemap measurements and a determination of epitaxial relationship with respect to the substrate, while the reflectivity measurements provide us information about the thickness, surface/interface roughness and density of single or multilavered structures on a substrate. The above-mentioned applications of the system are enabled by a sample stage with five computer-controlled and programmable axes and very powerful 2D area detector, capable of measuring in the OD mode (standard point detector), 1D mode (fast linear detector) and 2D mode (area detector). In addition to a structural characterization of thin films, standard powder-diffraction measurements can also be performed, optionally with a diffracted beam monochromator for sample fluorescence removal. Furthermore, the system is equipped with high/low-temperature sample stages, which make it possible to measure samples over a broad temperature range from -261°C to 1200°C and in different gas atmospheres.



Figure 11: Empyrean X-ray diffraction system

observed in the patterns. When the target-substrate distance increases to 60 mm, a pure-phase $Ag(Nb_{0.5}Ta_{0.5})O_3$ thin film is formed with the thickness of 150 nm, which nevertheless should be doubled for measuring the microwave dielectric properties. When the deposition time increases to 2 hours, a small concentration of $Ag_2(Nb_{0.5}Ta_{0.5})A_{0.21}$ secondary phase appears due to the decomposition of $Ag(Nb_{0.5}Ta_{0.5})O_3$ after long-time deposition. In the final part of the work, the repetition rate increases to 10 Hz and the deposition time is set at 1 hour to reduce the decomposition of $Ag(Nb_{0.5}Ta_{0.5})O_3$. In this way, a pure-phase polycrystalline $Ag(Nb_{0.5}Ta_{0.5})O_3$ thin film with a thickness of 300 nm is obtained.

In the scope of NAFERBIO project we investigated the synthesis of PMN-PT thin films. In short, we systematically varied the conditions of the reagents in order to determine the influence of the coordination chemistry on the formation of the perovskite phase. Results revealed that the major contribution to the formation of single-phase perovskite PMN-PT thin films comes from the coordination of the Pb reagent. A pyrochlore-free PMN-PT film with (100) orientation was formed when the steric hindrance of the Pb precursor was increased by using polyvinylpyrrolidone (PVP). The (111) orientated PMN-PT thin films were prepared using sol-gel-derived TiO₂ as a nucleation layer. Our research was further focused on the influence of the pyrolysis treatment on the phase formation and microstructural development of PMN-PT thin films. The XRD results showed that a different pyrolysis treatment has no influence on the phase formation of thin films. In contrast, the microstructural development of the PMN-PT thin films strongly depends on the used pyrolysis temperature.

Based on PMN-PT films with (100) orientation FBAR devices were subsequently fabricated and tested. Films were deposited on platinized silicon substrates. More than 4% tuning of resonance frequency under DC field less than 15 V/ μ m was demonstrated. In comparison with the Ba_xSr_{1x}TiO₃ based FBARs, this tunability was achieved at 2-3 times lower applied DC field. The other advantage of PMN-PT is the high electromechanical coupling coefficient that allows for development of wide-band tunable filters. Even though FBARs with this performance may be used in microwave circuits, the achieved tunability is not as high as we would anticipate from the large electrostriction coefficient of PMN-PT reported in the literature. In these experiments the lower electrostriction coefficient and lower tunability are due to the lower density of the PMN-PT films, which is the subject of forthcoming studies. An additional reduction of the tunability is due to large negative nonlinear electrostriction coefficient.

In addition, a part of our activities, in collaboration with an industrial partner, were focused on the development of aluminum foams. For such foams TiH_2 is used as a foaming agent. As an alternative forming agent we proposed in the past the application of dolomite. A drawback of the dolomite is its high decomposition temperature, which is above 820°C. In order to decrease its decomposition temperature we mechanically and chemically treated the dolomite and such products start to decompose at 400°C.

Within the cooperation with industrial partner Knauf Insulation d.o.o, the research work on the joint project was focused on the morphology and chemical composition of mineral fibres and their composites, crystallization and melting behaviour, aging process, determination of specific heat and thermal stability of mineral wools.

Organization of Conferences, Congresses and Meetings

 Workshop on MATERA ERA-NET project "Novel inorganic inks for hybrid printed electronic demonstrators", Ljubljana, 16. 10. – 17. 10.2013.

- Materials Science & Technology 2013 Conference and Exhibition, Montreal, Canada, 27. 10. – 31. 10. 2013 (co-organizers).
- 21st Conference on Materials and Technologies, Portorož, 13. 11. 15. 11. 2013 (coorganizers).
- 4. Institue of Science and Technology for Ceramics, Faenza, Italy and Institut "Jožef Stefan" Workshop on Materials, Ljubljana, 11. 12. – 12. 12. 2013.

Awards and Appointments

1. Aničić Nemanja: Award of the Henkel Slovenia Foundation for B. Sc. Thesis, Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, "Application of the population balance model for the prediction of concentrated emulsion droplet size distribution".

Patent granted

 Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, Composites materials based on ceramic phase and metal with functionalized surface as environmentally-friendly materials with antibacterial activity, a process for preparing and use thereof, SI24094 (A), Urad RS za intelektualno lastnino, 31.12.2013.

INTERNATIONAL PROJECTS

- 1. Thermoelectric Oxide Materials EPCOS OHG Ceramic Components Division Prof. Danilo Suvorov
- Microwave Tunable Materials, Composites and Devices NATO - North Atlantic Treaty Organisation Asst. Prof. Boštjan Jančar
- The Synthesis of Dielectric Materials by Chemical Solution Deposition and Characterization of their Dielectric Properties Slovenian Research Agency Prof. Danilo Suvorov
- Nanostructural Designing of Multifunctional and Sintered Electrical and Biological Functionally Graded Materials Slovenian Research Agency Asst. Prof. Srečo Davor Škapin
- Multifunctional Ferroelectric Materials based on Ag(Nb,Ta)O₃ Slovenian Research Agency Prof. Danilo Suvorov

RESEARCH PROGRAM

1. Contemporary Inorganic Materials and Nanotechnologies Prof. Danilo Suvorov

VISITORS FROM ABROAD

- Hermann Gruenbichler, B. Sc., Dr. Manfred Schweinzger, Dr. Yongli Wang, TDK EPCOS, Deutschlandsberg, Austria, 6. 3. 2013.
- Dr. Markus Mente, Gorazd Šebenik, B. Sc., Borut Vezočnik, B. Sc., Knauf Insulation, Škofja Loka, 9. 5. 2013.
- Prof. Dr. Dragoljub Uskoković, Institut of Tecnical sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, 16. 7. – 17. 7. 2013.
- Prof. dr. Ivan Sondi, Faculty of mining, geology and petroleum engineering, University of Zagreb, Zagreb, Croatia, 9. 4. 2013.
- Dr. Smilja Marković, Institut of Tecnical sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, 7. 6. – 19. 6. 2013.
- Dr. Jyoti Prosad Guha, Missoury University of Science and Technology, Rolla, USA, 10. 6. - 14. 8. 2013.
- Dr. Smilja Marković, Institut of Tecnical sciences of the Serbian Academy of Sciences and Arts, Belgrade, Serbia, 5. 8. – 14. 8. 2013.
- Prof. Dr. Suk-Joong L. Kang, Korea Advanced Institute of Science and Technology, Daejeon, South Korea, 28. 8. - 30. 8. 2013.
- 9. Dr. Hiroyuki Enomoto, Dr. Kesaku Sonoda, Research Laboratories of NOF Corporation, Tsukuba, Japan, 16. 10. – 17. 10. 2013.



Figure 12: New laboratory for antibacterial materials analysis

We established a new laboratory for the analysis of antibacterial materials, where we will be able to grow bacterial and mammalian cells and examine their survival after being exposed to the prepared materials as well as their interactions with these materials.

R&D GRANTS AND CONTRACTS

- 1. Nanoengineering of Self-Assembled Materials
- Prof. Danilo Suvorov
- New Materials for Power Conversion: Oxide Semiconductor Thermoelectrics
 Prof. Danilo Suvorov
- INNOINKS: Novel Inorganic Inks for Hybrid Printed Electronic Demonstrators Prof. Danilo Suvorov
- 5. NAFERBIO: Nanostructured Ferroelectric Films for Biosensor
- 6. Prof. Danilo Suvorov

NEW CONTRACTS

- Development and Characterisation of Mineral Wool Fibres Knauf Insulation, d. o. o., Škofja Loka Prof. Danilo Suvorov
- New Materials for Energy Conversion: Oxide Semiconducting Thermoelectrics Gorenje Household Appliances, d. d. Prof. Danilo Suvorov
- Prof. Dr. Heli Jantunen, Dr. Jari Juuti, Dr. Mikko Nelo, Dr. Tuomo Siponkoski, University of Oulu, Oulu, Finland, 16. 10. – 17. 10. 2013.
- 11. Prof. Dr. Malgorzata Jakubowska, Dr. Marcin Sloma, Institute of Electronic Materials Technology, Warsaw, Poland, 16. 10. – 17. 10. 2013.
- Dr. Carmen Galassi, Piezoelectric Materials Research Group, Institute of Science and Technologyfor Ceramics, Faenza, Italy, 11. 12. – 12. 12. 2013.
- Dr. Michele Iafisco, Bioceramics Research Group, Institute of Science and Technologyfor Ceramics, Faenza, Italy, 11. 12. – 12. 12. 2013.
- 14. Dr. Elisa Mercadelli, Dr. Alessandra Sanson, Materials Research Group, Institute of Science and Technology for Ceramics, Faenza, Italy, 11. 12. 12. 12. 2013.
- Dr. Damir Dominko, Dr. Damir Staresinić, Institute of Physics, Zagreb, Croatia, 19. 12. 2013.
- Dr. Maja Dekić, Amra Salčinović, Faculty of natural sciences and mathematics, University of Sarajevo, Sarajevo, Bosnia and Herzegovina, 19. 12. 2013.

Visiting researchers

- Dr. Ismael Fabregas, Centro de Investigaciones en Sólidos, CITEFA, Buenos Aires, Argentina, 1. 1. 2013 – 31. 8. 2013.
- Dr. Zoran Jovanović, Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, 1. 1. 2013 – 31. 12. 2013.
- 3. dr. Lei Li, Zhejiang University, Hangzhou, China, 1. 1. 2013 31. 12. 2013

STAFF

Researchers

- 1. Asst. Prof. Boštjan Jančar
- 2. Dr. Špela Kunej
- 3. Dr. Marjeta Maček Kržmanc
- Dr. Matjaž Spreitzer
 Prof. Danilo Suvorov, Head
- 6. Asst. Prof. Srečo Davor Škapin
- Postdoctoral associates
- 7. Dr. Jakob König
- 8. Dr. Manca Logar
- 9. Dr. Asja Veber
- 10. Dr. Marija Vukomanović
- Postgraduates
- 11. Nemanja Aničić, B. Sc.

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ORIGINAL ARTICLE

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12. Sonja Jovanović, B. Sc.

13. Dejan Klement, B. Sc.

14. Mario Kurtiak, B. Sc.

15. Mojca Otoničar, B. Sc.

17. Andreja Šestan, B. Sc.

20. Damjan Vengust, B. Sc.

21. Maja Šimaga, M. Sc.

18. Dr. Tina Šetinc, left 01.07.13

Technical and administrative staff

16. Tilen Sever, B. Sc.

19. Vojka Žunič, B. Sc.

Technical officer

22. Silvo Zupančič

- 13. Špela Kunej, Asja Veber, Danilo Suvorov, "Sol-gel synthesis and characterization of $Na_{0.5}Bi_{0.5}TiO_3 NaTaO_3$ thin films", *J. Am. Ceram. Soc.*, vol. 96, no. 2, pp. 442-446, 2013.
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PUBLISHED CONFERENCE CONTRIBUTION

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- 2. Sonja Jovanović, Matjaž Spreitzer, Mojca Otoničar, Danilo Suvorov, "The influence of oleic acid on the morphology and magnetic properties of CoFe₂O₄ nanoparticles", In: *Zbornik*, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 288-295.
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MONOGRAPH

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PATENT APPLICATION

1. Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, *Functionalized hydroxyapatite/gold composites as "green" materials with antibacterial activity and a process for preparing and use thereof*, W02013187846 (A1), World Intellectual property organization, 19.12.2013.

PATENT

1. Marija Vukomanović, Srečo D. Škapin, Danilo Suvorov, *Composites* materials based on ceramic phase and metal with functionalized surface as environmentally-friendly materials with antibacterial activity, a process for preparing and use thereof, SI24094 (A), Urad RS za intelektualno lastnino, 31.12.2013.

MENTORING

1. Tina Šetinc, Influence of synthesis methods on the functional properties of Na_{0.5}Bi0.5TiO₃ (NBT), SrTiO₃ (ST) and NBT-ST composite material: doctoral dissertation, Ljubljana, 2013 (mentor Danilo Suvorov; comentor 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 with respect to 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 of 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.



We have continued our work in the apoptosis field with a major focus on cysteine cathepsins. The cathepsins are normally found within the endolysosomal vesicles, which contain an arsenal of hydrolases, including proteases such as cysteine cathepsins, but if released to the cytosol can initiate apoptosis signalling pathways. Endogenous and exogenous compounds have been identified that can mediate the destabilization of lysosomal membranes. It was shown that lysosomal proteases are not only able to initiate apoptotic signalling, but can also amplify the apoptotic pathways initiated in other cellular compartments. The endocytic pathway also receives cargo destined for degradation via the autophagic pathway. By recycling energy and biosynthetic substrates, and by degrading damaged organelles and

molecules, the endocytic system assists the autophagic system in resisting apoptotic stimuli. In a critical review we have discussed steps leading to lysosomal membrane permeabilization and the subsequent triggering of cell death, as well as the therapeutic potential of intervention in lysosomal membrane permeabilization. We have also investigated the mechanism of action of the sigma-2 receptor agonist siramesine, which was shown to trigger the cell death of cancer cells and exhibit a potent anticancer activity *in vivo*. Initially, the compound was suggested to trigger lysosomal membrane permeabilization, but its mechanism of action remained poorly understood. We have

shown that siramesine can induce rapid cell death in a number of cell lines at concentrations above 20 µM. In HaCaT cells, cell death was accompanied by caspase activation, the rapid loss of mitochondrial membrane potential, cytochrome c release, cardiolipin peroxidation and typical apoptotic morphology, whereas in U-87MG cells most apoptotic hallmarks were not notable, although mitochondrial membrane potential was rapidly lost. In contrast to the rapid loss of mitochondrial membrane potential above 20 µM siramesine, a rapid increase in lysosomal pH was observed for all the concentrations tested, which was, however, not accompanied by lysosomal membrane permeabilisation and the release of lysosomal enzymes into the cytosol. The lipophilic antioxidant -tocopherol, but not the hydrophilic antioxidant N-acetyl-cysteine, considerably reduced the cell death and destabilisation of mitochondrial membranes, but did not prevent the increase in lysosomal pH. At low concentrations, siramesine triggered cell death after two days or later, which seems to be associated with a general metabolic and energy imbalance due to defects in the endocytic pathway, intracellular trafficking and energy production, and not by a specific molecular event. Overall, we have shown that cell death in siramesine-treated cells is induced by the destabilisation of Figure 1: Lung colonization of tumor cells after i.v. injection

In 2013, we set up the first whole-body imaging platform in Slovenia, based on the **IVIS Spectrum imaging system. This platform** enables fluorescence and bioluminescence imaging in small animals, including 3-D image reconstruction, which is critical for the evaluation of novel diagnostic and therapeutic tools, as well as for the identification of in vivo signalling pathways.



mitochondria and is independent of the lysosomal membrane permeabilisation and the release of cathepsins into the cytosol, which is important for the development of the next generation of siramesine analogues.

Further work, which at least partially involves cysteine cathepsins and cell death, was performed on the role of the endogenous inhibitor of cathepsins, stefin B, in cancer. To investigate its role in mammary cancer, stefin B null



Figure 2: Orthotopic transplantation of tumor cells into mammary gland

mice were crossed with transgenic mammary cancer model mice. We have shown that the ablation of stefin B resulted in the reduced size of mammary tumours, but did not affect their rate of metastasis. Importantly, the decrease in tumour growth was correlated with an increased incidence of dead cell islands detected in tumours of stefin B-deficient mice. An ex vivo analysis of primary mammary tumour cells revealed that upon treatment with the lysosomotropic agent Leu-Leu-OMe, cancer cells lacking stefin B exhibited a higher sensitivity to apoptosis. Moreover, stefin B-deficient tumour cells were significantly more prone to cell death under increased oxidative stress. These results indicate an in vivo role for stefin B in protecting cancer cells by promoting their resistance to oxidative stress and to apoptosis induced through the lysosomal pathway. In addition, several stefin B mutants, characteristic for a rare epilepsy form, were found to be partially unfolded, and thereby potential targets for proteolytic cleavages by cathepsins S and B. The co-localization of stefin B wild type and EPM1 mutants with cathepsins showed that the cathepsins accumulate around the aggregates formed by the mutants. We hypothesize that the aggregation of the full-length mutants prevents the cathepsins from accessing the substrate protein's core, whereas the cleaved fragments would be expected to aggregate more strongly. In addition to stefin B, also cathepsin F, a cysteine cathepsin with an unusual

cystatin domain in the prodomain was found to be linked with aggregation. Wild-type human cathepsin F was namely found to localize to lysosomes, whereas several of its N-terminally truncated forms were found to aggregate and accumulate within aggresome-like inclusions. These inclusions nicely co-localised with several autophagy markers, suggesting that autophagy is the major protective and prosurvival mechanism responsible for the clearance of the N-terminally truncated forms of human cathepsin F.

More work has been done on understanding protease function in health and disease. Osteoarthritis and rheumatoid arthritis are destructive joint diseases that involve the loss of articular cartilage with a potential implication of cysteine cathepsins. We have thus shown that stimulation of the cultivated chondrocytes with two cytokines, interleukin-1 α and/or tumour necrosis factor α , resulted in a time-dependent increase in cathepsin S expression and induced its secretion into the conditioned media. Using a novel bioluminescent activity-based probe, we were able to demonstrate a significant increase in proteolytic activity of cathepsin S in the conditioned media of proinflammatory cytokine-stimulated chondrocytes. Its stability at neutral pH and potent proteolytic activity on extracellular matrix components mean that cathepsin S may contribute significantly to cartilage degradation and may thus be considered a potential drug target in joint diseases.

We also worked on the identification of protease substrate specificities and on the development of proteomic methods for their identification. In collaboration with dr. M. Drag (University of Wroclaw) we determined, using



Figure 3: Schematic resentation of apoptotic signaling pathways and the role of lysosomes (after Repnik et al., 2013, CSH Perspectives in Biology 5, a008755)

combinatorial libraries of fluorescent substrates, that unnatural amino acids increase the activity and specificity of synthetic substrates for human and malarial cathepsin C, a finding that may have much wider applications, also to other proteases. In addition, with prof. dr. K. Gevaert (University of Ghent) we have been collaborating on the development of novel proteomic methods for substrate profiling, and introduced a new method for in-solution sample preparation using microfilter devices, combined with the use of the so-called stage-tip protocol, which was successfully tested on cathepsins. In addition, prof. dr. D. Turk has continued to develop the MAIN software, which has been designed to interactively perform the complex tasks of macromolecular crystal-structure determination and validation. Using MAIN, it is possible to perform density modification, manual and semi-automated or automated model building and rebuilding, real- and reciprocal-space structure optimization and refinement, map calculations and various types of molecular structure validation. Using MAIN, it is possible to optimize non-crystallographic symmetry parameters and envelopes and to refine the structure in single or multiple crystal forms.

We participated in two FP7 projects, being the coordinators of one of them (LIVIMODE). We were also involved in two Slovenian Centers of Excellence, Center for Integrative approaches for Chemistry and Biology of Proteins (CIPKEBIP) that we also coordinate, and Nanosciences and Nanotechnologies. We were partners in the competence center BRIN, which, similarl to both Centers of Excellence, brings together researchers from both industry and academia. In addition, there are numerous other international collaborations with excellent research teams from different countries including Belgium, France, Germany, Sweden, Switzerland, UK, USA, Australia and Japan, which resulted in joint publications.

Prof. dr. Vito Turk was elected as a member of Slovene Academy of Sciences and Arts (SAZU), whereas prof. dr. Boris Turk was elected as a member of Academia Europea (London). Several members of the department were invited to give lectures at international symposia and foreign universities.

Some outstanding publications in the past year

- 1. Repnik, U., Hafner Česen, M., Turk, B. (2013): The endolysosomal system in cell death and survival. Cold Spring Harb Perspect Biol. 5(1):a008755. doi: 10.1101/cshperspect.a008755
- 2. Hafner Česen, M., Repnik, U., Turk, V., Turk, B. (2013): Siramesine triggers cell death through destabilisation of mitochondria, but not lysosomes. Cell Death Dis. 4:e818. doi: 10.1038/cddis.2013, 361
- Butinar, M., Prebanda Trstenjak, M., Rajković, J., Jerič, B., Stoka, V., Peters, C., Reinheckel, T., Krüger, A., Turk, V., Turk, B., Vasiljeva, O. (2013): Stefin B deficiency reduces tumor growth via sensitization of tumor cells to oxidative stress in a breast cancer model. Oncogene, doi: 10.1038/onc.2013, 314
- 4. Turk, D. (2013): MAIN software for density averaging, model building, structure refinement and validation. Acta Crystallogr D Biol Crystallogr. 69, 1342–1357

Awards and appointments

1. Boris Turk: Member of Academia Europea, London, United Kingdom

Organization of conferences, congresses and meetings

1. 30th Winter School on Proteinases and Inhibitors, Tiers, Italy, 27. 2.-3. 3. 2013, coorganisers

Patent granted

1. S. G. Psakhie, Volia Isaevich Itin, D. A. Magajeva, O. G. Terehova, E. P. Najden, Olga Vasiljeva, Georgij Mihajlov Andrejevič, Urška Mikac, Boris Turk, Contrast agent for T1 and/or T2 magnetic resonant scanning and method for preparing it, RU2471502 (C1), Federal'naja služba po intellektual'n'noj so'stvennosti, 10.1.2013.

INTERNATIONAL PROJECTS

- 1. 7FP ALEXANDER; Mucus Permeating Nanoparticulate Drug Delivery Systems European Commission Asst. Prof. Olga Vasiljeva
- 7FP LIVIMODE; Light-based Functional in Vivo Monitoring of Diseases Related Enzymes
 - European Commission
 - Prof. Boris Turk
- 3. MD Simulations of the Initial Steps in Oligomerization of an Amyloidogenic Protein Human Stefin B; in Comparison to the Less Amyloidogenic Stefin A Slovenian Research Agency
 - Prof. Eva Žerovnik
- 4. Nuclear Inhibitors of Cysteine Proteinases Influence Heterochromatin Distribution in the Nucleus
 - Slovenian Research Agency
 - Asst. Prof. Nataša Kopitar Jerala
- The Role of Cystatins in Immune Response to Viruses Slovenian Research Agency Asst. Prof. Nataša Kopitar – Jerala
- Assi, Prof. Natisa Rophar Jeraia
 Protective role of cystatins in LPS induced oxidative stress and sepsis Slovenian Research Agency
 - Asst. Prof. Nataša Kopitar Jerala
- Cofinancing of promotion of science and functioning of international scientific associations European Commission
 - Prof. Boris Turk

RESEARCH PROGRAMS

- I. Structural Biology
- Prof. Dušan Turk
- 2. Proteolysis and Its Regulation Prof. Boris Turk

R&D GRANTS AND CONTRACTS

- 1. Cell Signalling of Toll-like Receptors
- Asst. Prof. Nataša Kopitar Jerala 2. Secretory Vesicle Mobility and Calcium Homeostasis in Astrocytes
- Prof. Veronika Stoka
 Study of Hom(e)ologous Recombination in the Evolution of Polyketide Synthases
 Prof. Boris Turk
- 4. The Role of Small GTPases in the Regulation of Endosomal/Lysosomal Transport in Astrocytes
- Prof. Veronika Stoka5. Nitroxoline and Its Derivatives as New Antitumour Drugs Asst. Prof. Olga Vasiljeva
- Asst. Prof. Olga vasileva
 The Role of Cysteine Cathepsins in Cellular Signalling Prof Boris Turk
- Role and Relevance of Empirical Geometric Parameters in Crystal Structure Determination of Macromolecules for Prediction of Ligand Binding Prof. Dušan Turk



- Involvement of the Lysosomal Cysteine Peptidase Inhibitors in Progression and 8 Metastasis of Mammary Cancer Asst. Prof. Olga Vasiljeva
- 9 Inhibitors of Cysteine Carboxypeptidases as Regulators of Autoimmune and Neurodegenerative Processes Asst. Prof. Olga Vasiljeva
- 10. Oligomers of Amyloidogenic Proteins from A to Z: Biophysical Properties, Structure, Function and Mutual Interactions Prof. Eva Žerovnik

VISITORS FROM ABROAD

- Georgy Mikhaylov, Siberian State Medical University, Tomsk, Russia, 1. 1.-31. 12. 2013 1. (IJS fellowship holder)
- Andrey Kadin, Shemyakin and Ovchinnikov Institute of Bioorganic Chemistry, Russian 2 Academy of Science, Moscow, 1. 1.-31. 12. 2013 (IJS fellowship holder)

- 11. Role of Cysteine Pproteases in the Process of Cancerogenesis Asst Prof Marko Fonović
- 12. Research on New Technologies for Conservation Restoration of Baroque Easel Paintings Asst. Prof. Marko Fonović
- Use of Adipose-derived Stem Cells for Engineering Vascularized Tissue Implants 13. Dr. Mirjam Fröhlich
- 14 Competency Centre for Biotechnological Development and Innovation: CC BDI Prof. Boris Turk
- 3 Prof. Kazuo Umezawa, Department of Molecular Target Medical Screening, School of Medicine, Aichi Medical University, Nagakute, 20.-21. 9. 2013
- 4 Prof. Kris Gevaert, VIB Department of Medical Protein Research, UGent Proteome Analysis and Bioinformatics Unit, Gent, Belgium, 14.-15. 11. 2013

STAFF

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- 24. Dr. Aleksandra Usenik
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ORIGINAL ARTICLE

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REVIEW ARTICLE

- 1. Marko Novinec, Brigita Lenarčič, "Cathepsin K: a unique collagenolytic cysteine peptidase", *Biol Chem*, vol. 394, no. 9, pp. 1163-1179, 2013.
- Marko Novinec, Brigita Lenarčič, "Papain-like peptidases: structure, function, and evolution", *Biomol. concepts*, vol. 4, issue 3, pp. 287-308, 2013.

PUBLISHED CONFERENCE CONTRIBUTION

- Nevenka Kregar-Velikonja, Ariana Barlič, Mirjam Fröhlich, Miomir Knežević, "Gojenje hondrocitov za zdravljenje poškodb sklepnega hrustanca", In: Sodobni pristopi pri zdravljenju s krvjo, celicami in tkivi: zbornik z recenzijo, Cvetka Gregorc, ed., Ljubljana, Zbornica zdravstvene in babiške nege Slovenije - Zveza društev medicinskih sester, babic in zdravstvenih tehnikov Slovenije, Sekcija medicinskih sester in zdravstvenih tehnikov v anesteziologiji, intenzivni terapiji in transfuziologiji, 2013, pp. 52-58.
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INDEPENDENT COMPONENT PART OR A CHAPTER IN A

Monograph

- Antonio Baici, Marko Novinec, Brigita Lenarčič, "Kinetics of the interaction of peptidases with substrates and modifiers", In: *Proteases: structure and function*, Klaudia Brix, ed., Walter Stöcker, ed., Wien, Springer-Verlag, cop. 2013, pp. 37-84.
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- 3. Nataša Kopitar-Jerala, "Cysteine proteinase Inhibitors in the nucleus and nucleolus in activated macrophages", In: *Proteins of the nucleolus regulation, translocation, & biomedical functions*, Danton H. O'Day, ed., Andrew Catalano, ed., [S. l.], Springer, 2013, pp. 305-322.
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PATENT APPLICATION

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PATENT

1. S. G. Psakhie, Volia Isaevich Itin, D. A. Magajeva, O. G. Terehova, E. P. Najden, Olga Vasiljeva, Georgij Mihajlov Andrejevič, Urška Mikac, Boris Turk, *Contrast agent for T1 and/or T2 magnetic resonant scanning and method for preparing it*, RU2471502 (C1), Federal'naja služba po intellektual'n'noj so'stvennosti, 10.1.2013.

Mentoring

- 1. Maruša Hafner Česen, *The effect of siramesine on cell death pathway and comparison to other lysosomotropic reagents:* doctoral dissertation, Ljubljana, 2013 (mentor Vito Turk; co-mentor Boris Turk).
- Marina Klemenčič, Role of the SMOC-1 and SMOC-2 proteins in extracellular matrix: doctoral dissertation, Ljubljana, 2013 (mentor Brigita Lenarčič).
- 3. Mira Polajnar, *Gain of toxic and loss of normal functions of human stefin B EPM1 mutants:* doctoral dissertation, Ljubljana, 2013 (mentor Eva Žerovnik).

DEPARTMENT OF MOLECULAR AND **R-2 BIOMEDICAL SCIENCES**

The research program of the Department of Molecular and Biomedical Sciences is focused mainly on basic research in protein biochemistry, molecular and cellular biology, and genetics. The primary goal of our investigations is the acquisition of a new understanding of mammalian pathophysiology with the aim of improving human and animal health.

Secreted phospholipases A,

One of the major research topics of the department is secreted phospholipases A, (sPLA,s) originating from animal toxins as well as those found in humans. We are studying the molecular mechanisms of action of the toxic sPLA₃s, particularly those endowed with presynaptic neurotoxicity, and the role of endogenous sPLA,s in pathological and physiological processes in mammals.

We have been invited to prepare a review for a monograph entitled "Genetic Manipulation of DNA and Protein - Examples from Current Research" (T. Petan et al., InTech Open Access, (2013), 107-132). In this overview, our successful protein-engineering approach in the structure-function studies of sPLA,s from viperid venoms was presented. Head:

By developing innovative procedures to renature recombinant sPLA,s we tried to obtain an enzymatically Prof. Igor Križaj inactive form of ammodytoxin A (AtxA), a neurotoxic sPLA, from the venom of the nose-horned viper (Vipera ammodytes ammodytes). The results are encouraging, and we expect that we will be able to produce a sufficient amount of the correctly folded protein in the next year. This will enable an accelerated characterization of novel sPLA, receptors, an advance in the study of the translocation mechanisms of these molecules through a plasma membrane and between different compartments in the cell, as well as intracellular trafficking of the sPLA, in real time. We study the molecular mechanism of action of presynaptically neurotoxic sPLA,s also using OS, from the venom of the Australian taipan (Oxyuranus scutellatus scutellatus). AtxA and OS, are structurally different sPLA,s. The first belongs to the group II, and the second to the group I sPLA,s. As model molecules, they are therefore complementary. The identification of an sPLA, receptor in the presynaptic membrane of a motoneuron (N-sPLA,R), which is crucial for the expression of neurotoxicity, has been a large research challenge already for many years. OS, binds to this receptor with an affinity 1000-fold higher than that of AtxA; therefore, it represents an ideal ligand for the study of N-sPLA, R. Following the preparation of large quantities of the recombinant wild-type OS, and its chimera with similar, but non-toxic, OS,, from the venom of the same snake, we continued in 2013 the collaboration with a research group from the Institute of Molecular and Cellular Pharmacology of the National Centre for Scientific Research (CNRS), Valbonne, France, in the scope of an international bilateral project Proteus, by developing a procedure for the preparation of the photo-reactive derivatives of these sPLA_s. The derivatives are currently being characterized.

sPLA,s represent a physiologically very important family of multifunctional proteins, whose effects do not depend solely on their enzymatic activity but, in some cases, also on their ability to bind to other molecules. We have been searching for new sPLA2-binding molecules using immuno-affinity

chromatography. In this way, we identified an Atx-binding protein in the venom of the nose-horned viper, which inhibited the activity of chymotrypsin (ChI), structurally belonging to the Kunitz-type proteinase inhibitors. Interestingly, the first results show that the toxicity of AtxA is increased in the presence of ChI. ChI-like molecules are present in mammals. It will be interesting to analyse the affinity of these molecules to sPLA,s and the physiological consequences of their interaction with sPLA, (M. Brgles et al., Analytical and Bioanalytical Chemistry, in press).

Following demonstrations that sPLA_ss can also act inside cells, we continue to study the intracellular activities of these molecules using different cellular models. In 2013 we tested the hypothesis of the molecular mechanism of AtxA action, based on our results obtained on the yeast Saccharomyces cerevisiae, by which AtxA inhibits endocytosis, on a mammalian cellular model, the isolated mouse neuromuscular junction. By characterising an enzymatically active mutant of the catalytically inactive, non-neurotoxic ammodytin L (AtnL), AtnL-LW, we also confirmed the validity of the model in mammalian cells. Restoration of the enzymatic activity conferred to AtnL both the ability to inhibit endocytosis in yeast and to act as a presynaptically neurotoxic sPLA, at the mammalian neuromuscular junction (N. Vardjan et al., Communicative and Integrative Biology, 6 (2013), e23600).

We studied the intracellular action of Atx also on mammalian cell lines, murine NSC34 and rat PC12. We performed a confocal-microscopy study of the translocation dynamics of Atx into PC12 cells. Using the same technique,



New substances and molecular tools to improve human and animal health.



Figure 1: Human group X sPLA₂ induces triacylglycerol synthesis and lipid droplet (LD) formation in MDA-MB-231 cells in an enzymatic activity-dependent manner. The cells were grown in a complete culture medium in the presence of 1 nM hGX for 48 h, fixed, stained with Nile red to visualise the LDs (green) and DAPI to visualise the nuclei (blue). Note a significant increase in the amount of LDs in hGX-treated cells in comparison with a non-treated control. The figure is reproduced from A. Pucer et al., Molecular Cancer, 12 (2013), e111.



Figure 2: Comparative display of the interacting areas between subunits in VaH3 and VaH4. In the case of VaH3, a disulphide bond between the subunits forms between two Cys176 residues. In the case of VaH4, an intra-subunit disulphide bond is formed, however, between two Cys132 residues. Therefore, P-IIIc SVMP can be divided into two groups, one possessing a Cys132–Cys132 and the other a Cys174–Cys174 intrasubunit disulphide bond connection. The figures are reproduced from T. Sajevic et al., Biochimie, 95 (2013), 1158–1170 in A. Leonardi et al., Toxicon, 77 (2014), 141–155.



Multi-Trait Industrial Strain

Figure 3: Metabolic engineering and industrial biotechnology are expected to gain a lot using the transfer of genetic modules into industrial microorganisms. we determined the level of co-localization between Atx and mitochondria, as well as Atx and several intracellular proteins, following the internalisation of Atx into PC12 cells. The results are prepared for publication.

We published a paper clearly demonstrating that ammodytoxins efficiently release arachidonic acid (AA) and induce apoptosis in a motoneuronal cell line in an enzymatic activity-dependent manner (Z. Jenko-Pražnikar et al., NeuroToxicology, 35 (2013), 91-100). The role of sPLA, enzymatic activity, including AA release, in the induction of motoneuronal apoptosis has been studied by AtxA and homologous recombinant sPLA, s with different enzymatic properties. We analysed the effects of an AtxA(V31W) mutant with a very high enzymatic activity, enzymatically inactive S49-sPLA, (AtnL), its mutant with restored enzymatic activity (AtnL-LW), and non-toxic, enzymatically active sPLA, (AtnI₂). The addition of AA, AtxA, AtxA(V31W) and AtnL-LW, but not AtnL and AtnI₂, to motoneuronal cells resulted in caspase-3 activation, DNA fragmentation and disruption of the mitochondrial membrane potential, leading to a significant and rapid decrease in motoneuronal cell viability that was not observed in (control) mouse myoblast and human embryonic kidney cells. AtxA, AtxA(V31W) and AtnL-LW, but not AtnL and AtnI,, also liberated large amounts of AA specifically from motoneuronal cells, and this ability correlated well with the ability to induce apoptotic changes and decrease cell viability. The enzymatic activity of AtxA and similar sPLA,s is thus necessary, but not sufficient, for inducing motoneuronal apoptosis. These results suggests that specific binding to the motoneuronal cell surface, followed by internalisation and the enzymatic activity-dependent induction of apoptosis, possibly as a consequence of both extensive extra- and intracellular AA release, is necessary for Atx-induced motoneuronal cell death.

In 2013 a postdoctoral research project was concluded in the scope of which a detailed structural analysis of the interaction between Atx and calmodulin (CaM) has been studied by protein NMR spectroscopy. CaM is a regulatory protein in the cell cytosol, presumably very important for the intracellular activity of Atx and homologous mammalian $sPLA_2s$. Understanding on the atomic level of its interaction with $sPLA_2s$, as well as of the interaction of the $sPLA_2$ -CaM complexes with the phospholipid membrane, is very important for designing the regulation of these interactions. In collaboration with two partner groups, the Bijvoet Centre from the Utrecht University, the Netherlands, and the NMR centre from the National Institute of Chemistry in Ljubljana, we finished with the planned experimental work. The data processing and the preparation of publications are underway.

Aiming to dynamically observe the interaction between Atx and CaM in cells using a FRET method, we continued the development of fluorescent derivatives of both proteins.

In an attempt to formulate a protocol for the preparation of an effective antiserum against the nose-horned viper venom, we discovered that the quantity of Atx in the venom positively correlates with the level of venom immunogenicity. A rapid and accurate method for the quantification of Atx in the venom is therefore one of the key steps in preparing the antisera of a high quality. Together with colleagues from the Institute for Chemical Technologies and Analytics, Vienna University of Technology, we made another step forward in the efficient quantification of Atx in the venom. We developed an original method that is able to separate, in a single step, all three highly similar Atx isoforms (V.U. Weiss et al., *Electrophoresis*, in press).

It has been shown that nine active sPLA₂ enzymes known in humans display different tissue expression patterns and specific enzymatic preferences for binding to different types of phospholipid membranes, suggesting distinct biological roles for each sPLA₂. The multitude of cellular effects of the released free fatty acids (FFAs) and lysophospholipids, and of their numerous bioactive metabolites, further explain their involvement in a variety of physiological processes and diseases, including lipid digestion and remodelling, acute and chronic inflammatory diseases, cardiovascular diseases, reproduction and host defence against infections. Recent studies have confirmed that various sPLA₂s also play a significant role in cancer and metabolic disorders. For example, a few years ago, it was demonstrated that the human group X (hGX) sPLA₂ stimulates colon-cancer cell proliferation by a mechanism dependent on the released FFAs and lysophospholipids, but not on its potent stimulation of prostaglandin E₂ synthesis. The underlying mechanisms of the action of hGX sPLA, and other sPLA, enzymes in different cancers have not been

known and confirmations of their functional contribution to tumorigenesis have been waiting for additional studies. In 2013, we successfully completed and published an extensive study, using multiple breast-cancer cellular models, analysing the effects of hGX sPLA₂ on breast-cancer cell growth and survival in details, with an aim to better understand its mechanism of action (Pucer et al., Molecular Cancer, 12 (2013), e111). We were able to show for the first time that hGX sPLA, induces lipid droplet (LD) formation in the highly tumorigenic MDA-MB-231 breast-cancer cells (Figure 1) in an enzyme activity-dependent manner, thereby stimulating cell proliferation and significantly prolonging cell survival under serum deprivation-induced stress. Our results suggested that FFAs, in particular oleic acid, released from membrane phospholipids by the action of hGX sPLA₂, are substantially responsible for the LD biogenesis and cell survival. We also demonstrated that the mechanism of hGX-induced cell survival and lipid accumulation is associated with alterations in the expression of key lipogenic and β -oxidation enzymes, and the modulation of AMP-activated protein kinase (AMPK) and protein B/Akt kinase signalling pathways. The pro-tumorigenic effects induced by hGX sPLA, were abolished by etomoxir, suggesting a critical role for β-oxidation in hGX-induced LD formation and cell survival in breast-cancer cells. The ability of hGX sPLA, to act as a modulator of basic lipid metabolism and cancer cell survival is thus well established. This could have important implications in elucidating the role of hGX and other sPLA_ss, such as hGV and hGIII, in cancer and human pathophysiology in general.

The experience of our group in the field of sPLA₂ is also evidently well known to the editors of *Protein and Peptide Letters*, as they invited us to prepare a review article on the role of these molecules in the mammalian immune system (I. Križaj, *Protein and Peptide Letters*, in press).

Other pharmacologically active components from natural toxins

In 2013 we continued to systematically analyse the components of the nose-horned venom that affect the blood-coagulation process – haemostasis. We succeeded in publishing a description of one of the most haemorrhagic molecules from the venom, homodimeric metalloproteinase (SVMP) VaH3 (T. Sajevic et al., *Biochimie*, 95 (2013), 1158–1170). We also concluded with the experimental work on a heterodimeric, haemorrhagic SVMP, VaH4, and published these results (A. Leonardi et al., *Toxicon*, 77 (2014), 141–155). A very important conclusion stems from our analysis: in P-III class of SVMPs, dimers can be formed by a covalent inter-subunit crosslinking of either two

Cys132 or two Cys174 residues (Figure 2). Due to our achievements in the field of haemostatically-active components from snake venoms and connected pathologies we have been invited to submit a review article (T. Sajevic et al., *Toxin Reviews*, in press). In collaboration with our colleagues from the Institute of Immunology in Zagreb, Croatia, and the Vienna University of Technology we described another very interesting molecule from the venom of the nose-horned viper, a serine proteinase VaSP1 with the unconventional active site structure (T. Kurtović et al., *Toxicon*, 77 (2014), 93–104). Regarding the substrate specificity of this enzyme and the fact that it prolongs the prothrombin and activated partial thromboplastin times, it is very likely that it acts as anticoagulant.

High-throughput genetics and functional genomics in yeast Saccharomyces cerevisiae

Neonicotinoid insecticides were notorious in 2013 because of their proposed toxicity for bees and other nontarget organisms, on the basis of which they were banned in the EU in April 2013. Using chemogenomics analysis in the yeast model we have determined the side effects of neonicotinoid insecticides, and especially of additives from



Figure 4: Mechanisms involved in the process of the retroelement-derived domesticated gene (RDDG) neofunctionalisation. In the transition phase from retroelement remains to the first RDDGs, many nucleotide changes were necessary for the neofunctionalisation. One of the crucial steps in the process of neofunctionalisation was the exonisation of retroelement domains (Gag, protease, and integrase), which produced ready-to-use modules. Retroelement remains in mammalian genomes will normally turn into pseudogenes, due to lack of a promoter, and they can survive as a functional gene only if they recruit a new promoter sequence. To become expressed at a significant level and in the tissues where it can exert a selectively beneficial function, a new gene needs to acquire a core promoter and other structural elements that regulate its expression. Exons and introns are shown as orange (5' and 3'untranslated regions - UTRs) or grey (coding part of the exons) boxes and connecting lines. A de novo acquired promoter is shown in blue. The figure is reproduced from J. Kokošar and D. Kordiš, Molecular Biology and Evolution, 30 (2013), 1015-1031.

insecticide formulations. We have shown examples where the additives are even more toxic than the neonicotinoids themselves (M. Mattiazzi Ušaj et al., *Chemosphere*, in press).

In the field of genetics, the last years have seen a rapid development of techniques and methods for polygenic traits analysis, which have been spurred by recent developments in genomics. In our group we have been developing new experimental approaches and computational tools that will enable the transfer of combinations of genes (*i.e.*, genetic modules) in industrial microorganisms (Figure 3), which will revolutionise the field of metabolic engineering and industrial biotechnology.

The regulation of cellular processes through internal metabolic intermediates is one of the most exciting areas of molecular biology, which should contribute to new treatments for cancer, type-2 diabetes and neurodegenerative diseases. Acetyl-CoA is the key metabolite that broadly affects cellular processes. In 2013 we have finished our multiyear study on the regulation of cellular metabolism through a peroxisomal protein Pex11. We established that



Figure 5: Diverse sources of the retroelement-derived domesticated gene (RDDG) promoters. Various scenarios that lead to the transcription of RDDG copies are illustrated. (A) Recruitment of proto-promoters from the CpG island-less region. (B) Recruitment of proto-promoters from the CpG-rich island. (C) Recruitment of a bidirectional (CpG-enriched) promoter from neighbouring gene in the vicinity of the RDDG. (D) Recruitment of distant promoters in the genomic neighbourhood by the acquisition of a new 5'untranslated (UTR) exon-intron structure. (E) Sharing of the unidirectional (CpG-enriched) promoter from a neighbouring gene in the vicinity of the RDDG. Exons and introns are represented by orange and grey (RDDGs) or black (neighbouring genes in the case of bidirectional promoters) boxes and connecting lines. Distances between exons are not to scale. The figure is reproduced from J. Kokošar and D. Kordiš, Molecular Biology and Evolution, 30 (2013), 1015-1031.

Pex11 regulates the cytosolic concentration of acetyl-CoA, which makes Pex11 an interesting novel drug target.

Our colleague from the department, currently a postdoc at the University of Toronto, Canada, took part in the preparation of a review article about the contribution of the functional genomics and high-throughput methods to the studies of the cell polarity in yeast (E. Styles et al., *Philosophical Transactions of the Royal Society B Biological Sciences*, 368 (2013), 20130118).

Evolutionary genomics and study of retrotransposons

Vertebrates, especially mammals, possess numerous single-copy domesticated genes (DGs) that originated from the intronless multicopy transposable elements. However, the origin and evolution of the retroelement-derived DGs (RDDGs) that originated from Metaviridae has only been partially elucidated, due to the absence of genome data or a limited analysis of a single family of DGs. We traced the genesis and regulatory wiring of the Metaviridae-derived DGs through phylogenomic analysis, using whole-genome information from more than 90 chordate genomes (J. Kokošar and D. Kordiš, Molecular Biology and Evolution, 30 (2013), 1015–1031). Phylogenomic analysis of these DGs in chordate genomes provided direct evidence that major diversification has occurred in the ancestor of placental mammals. Mammalian RDDGs have been shown to originate in several steps by independent domestication events and to diversify later by gene duplications. An analysis of syntenic loci has shown that diverse RDDGs and their chromosomal positions were fully established in the ancestor of placental mammals. By an analysis of active Metaviridae lineages in amniotes, we have demonstrated that RDDGs originated from retroelement remains. The chromosomal gene movements of RDDGs were highly dynamic only in the ancestor of placental mammals. During the domestication process, de novo acquisition of regulatory regions is shown to be a prerequisite for the survival of the DGs (Figure 4). The origin and evolution of *de nov* o acquired promoters (Figure 5) and untranslated regions in diverse mammalian RDDGs have been explained by a comparative analysis of orthologous gene loci. The findings of this study thus provide a new view on the origin and evolution of the *de novo* acquired promoters, 5'- and 3'-UTRs in diverse mammalian RDDGs. The regulatory wiring of DGs and their rapid fixation in the ancestor of placental mammals have played an important role in the origin of their innovations and adaptations, such

as placenta and newly evolved brain functions. DGs could thus constitute an excellent system on which to analyse the mechanisms of regulatory evolution in placental mammals.

In 2013 we participated in a study led by our colleagues from the Faculty of Chemistry and Chemical Technology, University of Ljubljana (UL), about the way in which the APOBEC3 proteins inhibit the multiplication of the L2-retrotransposon. Clarification of the mechanism of action of APOBEC3 proteins is very important as these proteins inhibit the multiplication of numerous retrotransposons and retroviruses, among them also the HIV virus (N. Lindič et al., *Retrovirology*, 10 (2013), e156).

Other subjects

In 2013 we also worked on several projects out of the thematic scope of our department.

We collaborated intensively with colleagues from the Department of Biology, the Biotechnical faculty (BF), UL, in the determination of the mode of action of lipid membrane pore-forming proteins from the mushroom Pleurotus ostreatus. With structural identification we participated at the conclusion that for the formation of the pore in membranes, rich in cholesterol and sphingomyelin, pleurotolysin B requires the presence of another protein, ostreolysin A (K. Ota et al., Biochimie, 95 (2013), 1855-1864). During the isolation of ostreolysin A from the mushroom an additional protein co-eluted. Structural analysis of this protein revealed the first example of a protein consisting of hemopexin repeats in yeast (K. Ota et al., Biochim. Biophys. Acta - Proteins and Proteomics, 1834 (2013), 1468-1473). Together with the same group we also prepared a review paper on the use of pore-forming toxins for the sensing and labelling of membrane microdomains (M. Skočaj et al., Current Medicinal Chemistry, 20 (2013), 491-501). A very important joint project with colleagues from the BF was dedicated to developing an original approach against bacterial infections. In the evolvement of the resistance of bacteria against antibiotics their SOS system is of a crucial importance. The key role in the bacterial SOS response is played by a complex formed between a single-stranded DNA (ssDNA) and two bacterial proteins, RecA and LexA. Based on the experimental data we built a tri-dimensional model of the complex ssDNA-RecA-LexA (Figure 6), which will enable the



Figure 6: Model of the LexA-RecA* three-dimensional structure. (A) Six intact LexA monomers (spherical representation, each in a different colour) are docked on two turns of the RecA* (shown as grey transparent surface). (B) LexA-RecA* complex rotated by 120° around vertical axis relative to the view in (A). LexA monomers are presented in cyan and RecA in grey. The N- and C-termini of the two RecA monomers are marked. One of the LexA monomers is encircled by a broken line. (C) Detailed view of the LexA-RecA* complex. The same LexA monomer as in (B) is encircled. LexA C- and N-terminal domains (CTD and NTD) are indicated. Nine successive RecA monomers (presented in yellow and orange) surround one monomer of LexA. Seven RecA protomers out of nine constitute the LexA-interaction interface. The figure is reproduced from L. Kovačič et al., Nucleic Acids Research, 41 (2013), 9901–9910.

targeted design of substances to prevent the development of bacterial resistance to antibiotics. We published our results in a very prominent journal (L. Kovačič et al., *Nucleic Acids Research*, 41 (2013), 9901–9910).

Together with our partners from the University Medical Centre Ljubljana, Department of Rheumatology, we improved the isolation protocol of two proteins from human serum that are vital for the diagnostics of the antiphospholipid syndrome (A. Artenjak et al., *Clinical and Developmental Immunology*, in press).

With colleagues from the Institute of Biochemistry, the Medical Faculty, UL, we demonstrated that the recombinant human eritropoetin (EPO) modulates the expression of some genes and stimulates the proliferation of the MCF-7 breast-cancer cells. We did not, however, observe a correlation between the level of expression of different EPO receptor isoforms and the invasiveness of the breast-cancer cells (N. Trošt et al., *Radiology and Oncology*, 47 (2013), 382–389).

We helped colleagues from the National Institute of Chemistry and the Centre of Excellence for Polymer Materials and Technologies (CE PoliMaT) with the microbiological testing of the antibacterial activity of macroporous polyurethane hybrid material with a high content of zinc and showed that it is highly bactericidal (G. Ambrožič et al., *Materials Research Bulletin*, 48 (2013), 1428–1434).

Some outstanding publications in the past year

- 1. Kokošar, J., Kordiš D. (2013): Genesis and regulatory wiring of retroelement-derived domesticated genes: a phylogenomic perspective. Mol. Biol. Evol. 30, 1015–1031
- Kovačič, L., Paulič, N., Leonardi, A., Hodnik, V., Anderluh, G., Podlesek, Z., Žgur-Bertok, D., Križaj, I., Butala, M. (2013): Structural insight into LexA-RecA* interaction. Nucleic Acids Res. 41, 9901–9910
- 3. Pucer, A., Brglez, V., Payre, C., Pungerčar, J., Lambeau, G., Petan, T. (2013): Group X secreted phospholipase A₂ induces lipid droplet formation and prolongs breast cancer cell survival. Mol. Cancer 12, e111
- Sajevic, T., Leonardi, A., Kovačič, L., Lang Balija, M., Kurtović, T., Pungerčar, J., Halassy, B., Trampuš-Bakija, A., Križaj, I. (2013): VaH3, one of the principal hemorrhage-inducing factors in *Vipera ammodytes ammodytes* venom, is a homodimeric P-IIIc metalloproteinase. Biochimie 95, 1158–1170
- Vardjan, N., Mattiazzi, M., Rowan, E.G., Križaj, I., Petrovič, U., Petan, T. (2013): Neurotoxic phospholipase A₂ toxicity model – an insight from mammalian cells. Commun. Integr. Biol. 6, e23600

Awards and appointments

1. Award of the Slovenian Research Agency for an exceptional scientific achievement in 2012 in Slovenia in the field of Biochemistry and Molecular Biology (*Conus consors* snail venom proteomics unveils functions, pathways and novel families involved in its venomic system)

INTERNATIONAL PROJECTS

- Structural Explanation of the High Increase in Enzymatic Activity of Secreted 1. Phospholipases A, in Complex with Calmodulin by High Resolution NMR Utrech University, Faculty of Science Dr. Lidija Kovačič
- Towards the Identification of N-type sPLA, Receptors 2. Slovenian Research Agency Prof. Iože Pungerčar
- Financial support for the preparation of the project application within the 7th 3. Framework Programme European Commission Prof. Igor Križaj

RESEARCH PROGRAM

1. Toxins and Biomembranes Prof. Igor Križaj

R&D GRANTS AND CONTRACTS

- Apoptotic Effects of Alkylpyridinium Compounds on Lung Adenocarcinoma Cells 1 Prof. Igor Križaj
- 2. Molecular Description of Lipid Membrane Changes in Disease Prof. Igor Križaj
- 3. Discovering Innovative Drugs for Regulation of Haemostasis by Venomics of the Vipera ammodytes Snake Prof. Igor Križaj
- Pathogenomics and Systems Biology of New Virulence Factors in Pathogenic Bacteria 4 Prof Dušan Kordiš
- Structural Explanation of the High Increase in Enzymatic Activity of Secreted Phospholipases A, in Complex with Calmodulin by High Resolution NMR Dr. Lidija Kovačič

NEW CONTRACT

1

Postgraduates

11. Vesna Brglez, B. Sc.

12. Minca Ferlin, B. Sc. 13. Jernej Oberčkal, B. Sc.

Technical officer

Igor Koprivec

18.

16. Mojca Brložnik, B. Sc.

Darja Žunič Kotar

Jerney Obereka, D. Sc.
 Anja Pucer, B. Sc., left 01.10.13
 Tamara Sajevic, B. Sc., left 01.10.13

Technical and administrative staff

Analyses Central Technological Library at the University of Ljubljana Prof. Igor Križaj

VISITOR FROM ABROAD

Dr. Gerard Lambeau, Institute de Pharmacologie Moleculare et Cellulare, Universite 1. Nice, Sophia Antipolis, France, 11.-19. 9. 2013

STAFF

Researchers

- Asst. Prof. Dušan Kordiš 1.
- Prof. Igor Križaj, Head
- Dr. Adrijana Leonardi 3.
- Prof. Uroš Petrovič 5 Prof. Jože Pungerčar

Postdoctoral associates

- 6. Dr. Janez Kokošar
- Dr. Lidija Kovačič, on postdoctoral leave since 01.10.13
- 8. Dr. Mojca Mattiazzi Ušaj
- Asst. Prof. Toni Petan 9.
- 10. Dr. Jernej Šribar

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ORIGINAL ARTICLE

- 1. Gabriela Ambrožič, Jernej Šribar, Srečo D. Škapin, Majda Žigon, Zorica Crnjak Orel, "An antibacterial macroporous polyurethane hybrid material with a high content of zinc ions: a template to uniform ZnO nanoparticles", Mater. res. bull., vol. 48, no. 4, pp. 1428-1434, 2013.
- 2. Iztok Dogša, Mojca Brložnik, David Stopar, Ines Mandić-Mulec, "Exopolymer diversity and the role of levan in Bacillus subtilis biofilms", PloS one, vol. 8, iss. 4, pp. 1-10, e62044, 2013.
- 3. Zala Jenko Pražnikar, Toni Petan, Jože Pungerčar, "Ammodytoxins efficiently release arachidonic acid and induce apoptosis in a motoneuronal cell line in an enzymatic activity-dependent manner", Neurotoxicology (Park Forest South), vol. 35, pp. 91-100, 2013.
- 4. Janez Kokošar, Dušan Kordiš, "Genesis and regulatory wiring of retroelement-derived domesticated genes: a phylogenomic perspective", Molecular biology and evolution, vol. 30, issue 5, pp. 1015-1031, 2013.
- 5. Lidija Kovačič, Nejc Paulič, Adrijana Leonardi, Vesna Hodnik, Gregor Anderluh, Zdravko Podlesek, Darja Žgur-Bertok, Igor Križaj, Matej Butala, "Structural insight into LexARecA interaction", Nucleic acids res., vol. 42, issue 21, pp. 9901-9910, 2013.
- 6. Nataša Lindič, Maruška Budič, Toni Petan, Binyamin A. Knisbacher, Erez Y. Levanon, Nika Lovšin, "Differential inhibition of LINE1 and

LINE2 retrotransposition by vertebrate AID/APOBEC proteins", *Retrovirology*, vol. 10, art. no. 156, pp. 1-16, 2013.

- 7. Katja Ota, Adrijana Leonardi, Miha Mikelj, Matej Skočaj, Therese Wohlschlager, Markus Künzler, Markus Aebi, Mojca Narat, Igor Križaj, Gregor Anderluh, Kristina Sepčić, Peter Maček, "Membrane cholesterol and sphingomyelin, and ostreolysin A are obligatory for poreformation by a MACPF/CDC-like pore-forming protein, pleurotolysin B", Biochimie (Paris), vol. 95, iss. 10, pp. 1855-1864, 2013.
- 8. Katja Ota, Miha Mikelj, Tadeja Papler, Adrijana Leonardi, Igor Križaj, Peter Maček, "Ostreopexin: a hemopexin fold protein from the oyster mushroom, Pleurotus ostreatus", Biochimica et biophysica acta, Proteins and proteomics, vol. 1834, no. 8, pp. 1468-1473, 2013.
- 9. Anja Pucer, Vesna Brglez, Christine Payré, Jože Pungerčar, Gérard Lambeau, Toni Petan, "Group X secreted phospholipase A2 induces lipid droplet formation and prolongs breast cancer cell survival", Mol. Cancer, vol. 12, art. no. 111, pp. 1-23, 2013.
- 10. Tamara Sajevic, Adrijana Leonardi, Lidija Kovačič, Maja Lang Balija, Tihana Kurtović, Jože Pungerčar, Beata Halassy, Alenka Trampuš-Bakija, Igor Križaj, "VaH3, one of the principal hemorrhagins in Vipera ammodytes ammodytes venom, is a homodimeric P-IIIc metalloproteinase", Biochimie (Paris), vol. 95, issue 6, pp. 1158-1170, 2013.

Annual Report 2013
- Erin Styles, Ji-Young Youn, Mojca Mattiazzi, Brenda J. Andrews, "Functional genomics in the study of yeast cell polarity: moving in the right direction", *Philosophical Transactions, Biological Sciences*, vol. 368, no. 1629, pp. 20130118-1-20130118-11, 2013.
- 12. Nina Trošt, Tina Stepišnik, Sabina Berne, Anja Pucer, Toni Petan, Radovan Komel, Nataša Debeljak, "Recombinant human erythropoietin alters gene expression and stimulates proliferation of MCF-7 breast cancer cells", In: Articles from 7th Conference of experimental and translational oncology, April, 20-24, 2013, Portorož, *Radiol. Oncol.*, vol. 47, no. 4, pp. 382-389, 2013.
- 13. Nina Vardjan, Mojca Mattiazzi, Edward G. Rowan, Igor Križaj, Uroš Petrovič, Toni Petan, "Neurotoxic phospholipase A₂ toxicity model: an insight from mammalian cells", *Communicative & integrative biology*, vol. 6, no. 3, pp. 23600-1-23600-3, 2013.

REVIEW ARTICLE

1. Vasja Progar, Uroš Petrovič, "Vpliv parametrov sekvenciranja naslednje generacije na zanesljivost rezultatov v metagenomskih študijah", *Informatica medica slovenica*, vol. 18, no. 1/2, pp. 1-8, 2013.

 Matej Skočaj, Biserka Bakrač, Igor Križaj, Peter Maček, Gregor Anderluh, Kristina Sepčić, "The sensing of membrane microdomains based on pore-forming toxins", *Curr. med. chem.*, vol. 20, no. 4, pp. 491-501, 2013.

INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Toni Petan, Petra Prijatelj, Jože Pungerčar, "Protein engineering in structure-function studies of viper's venom secreted phospholipases A₂", In: *Genetic manipulation of DNA and protein - examples from current research*, David Figurski, ed., Rijeka, InTech, cop. 2013, pp. 107-132.

MENTORING

1. Janez Kokošar, *Comparative genomics and phenotypic impact of novel retrotransposon-derived genes in placental mammals:* doctoral dissertation, Ljubljana, 2013 (mentor Dušan Kordiš).

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 of the environment in which we live. Our research work is focused on the processes of cancer progression and immune response, neurodegenerative processes, the biology of fungi, plant stress response and on the search for new biotechnological approaches and products.

In 2013 the field of research on fungal protease inhibitors broadened our knowledge on trypsin inhibitors from mushrooms. We have shown that stable trypsin inhibitors are present in different edible and poisonous mushrooms. We have isolated and biochemically characterized trypsin inhibitors from the parasol mushroom (Macrolepiota procera), death cap (Amanita phalloides), and the honey fungus (Armillaria mellea). Their properties resemble Head: those of the previously characterized trypsin inhibitors cnispin and cospin from the mushrooms clouded agaric Prof. Janko Kos (Clitocybe nebularis) and the inky cap (Coprinopsis cinerea). They show exceptional stability, as even after heating to 100°C they still retain their inhibitory activity. Furthermore, we have previously reported that inhibitors of cysteine proteases, macrocypins from the parasol mushroom (Macrolepiota procera), exhibit a negative effect on the growth and development of Colorado potato beetle larvae, and in 2013 we have described their mechanism

of action in this process. The exceptional feature of these fungal protease inhibitors is that macrocypins do not elicit an adaptive response in the guts of Colorado potato beetle larvae to increased levels of protease inhibitors in food, which has been routinely shown for protease inhibitors from different animal and plant sources. Therefore, our results have been published in the Journal of Agricultural and Food Chemistry, which is the top journal in the subject category of Agriculture.

Macrocypins from the parasol mushroom (Macrolepiota procera), exhibit a negative effect on the growth and development of Colorado potato beetle larvae and do not elicit an adaptive response.

In the field of glycobiology, we continued with studies on different lectins from the mushrooms clouded agaric (Clitocybe nebularis) and the parasol mushroom (Macrolepiota procera). In addition to a biochemical characterization, where recombinant versions prepared in bacterial expression system were used, we focused on an analysis of their effects on different cell lines with an emphasis on immune cells. Additionally, we have in the field of lectin research performed an applicative project for an industrial partner.

In cooperation with the National Institute of Biology we have explored mushrooms as a novel source of proteins with antibacterial activity. We used a phytopathogenic Gram negative bacterium Ralstonia solanacearum as a model, which is the causative agent of a quarantine brown rot disease of potatoes and other economically important plants, including tomato, ginger, tobacco and banana plants. From the screening of 150 aqueous extracts from mushrooms collected in Slovenian forests, we have detected antibacterial activity in eleven. Three of those - from mushrooms soap-scented toadstool (Tricholoma saponaceum), velvet bolete (Suillus variegatus) and trooping funnel (Clitocybe geotropa) - caused slower progression of disease symp-



Figure 1: Testing of mushroom extracts on phytopathogenic Gram negative bacterium Ralstonia solanacearum

toms and lower disease occurrence in both tomato and potato plants. We described the preparation and content of extracts from selected mushroom species that showed antibacterial activity against the economically important bacterial phytopathogenic crop pest in a patent application "Composition and method for plant protection", filed at the Slovenian Intellectual Property Office (P-201300349).

We contributed a chapter entitled Medicinal Mushrooms, which represents the first complete presentation of medicinal mushrooms in the Slovenian literature, to a book published by the Slovenian Pharmaceutical Society

"Contemporary Phytotherapy", which is the first Slovenian book on medicinal plants, which is based only on scientifically supported research and clinical studies and is entirely the work of Slovenian authors. The book is an important source of information for specialists and students, but also for

Cysteine protease cathepsin X regulates neuroprotective function of gamma enolase.



Figure 2: A: Honey mushroom (Armillaria mellea) as a source of trypsin inhibitors

the users of medicinal plants who are interested in more detailed, scientifically supported data.

The continuing study of the response of the common bean (Phaseolus vulgaris) to drought has been directed to the aminopeptidases previously shown to be involved. Their activities in leaves change under the influence of stress, although to different extents. Interestingly, the pattern of these changes depends on the age and/or the position of the leaves. Two of these aminopeptidases have been classified as serine proteases, and others are dependent on metal ions, although they are also inhibited by serine protease inhibitors. Two of the latter enzymes hydrolyse Ala-AMC and Lys-AMC and are expressed in leaves and seedlings. The activity of the enzyme expressed in leaves is modulated by metal ions in the nanomolar/picomolar range. Mn2+ is the most likely candidate for the physiological activation of the enzyme activity of "leaf" aminopeptidase. In addition, a serine endopeptidase and several aminopeptidases, already shown to be involved in the response to complete desiccation of the model resurrection plant Ramonda serbica, have been characterised.

An important part of our research was focused on the role of proteases and protease inhibitors in malignant, immune and neurodegenerative processes. Within the programme group we determined molecular mechanisms that imply the role of cysteine protease cathepsin X in neurodegenerative and malignant processes. We also continued studies on the role of the cysteine protease inhibitor cystatin F in the regulation of dendritic cells and natural killer cells (NKs). In the latter we demonstrated that the mechanism leading to its monomeric active form in endosomes/

Overexpression of the protein FUS is associated with amyotrophic lateral sclerosis.



Figure 3: The structure of lectin MpL

lysosomes, significantly affects the activity of the cathepsins C and H and consequently the cytotoxicity of NK cells. The activity of cystatin F seems to be crucial for the split anergy of NK cells, a mechanism caused by tumour cells to avoid their destruction.

We continued our research on the role of FUS protein in the frontotemporal dementia (FTD) and amyotrophic lateral sclerosis (ALS). We reported that overexpression of the wildtype FUS protein in a mouse model leads to symptoms similar to ALS. The resulting mouse model will enable more detailed studies of the mechanisms of the disease, as well as the testing of new therapeutic approaches. The results were published in Acta Neuropathologica. In a study published in Human Molecular Genetics we found that the disease associated mutations in FUS prevent its entry into the cell nucleus, giving rise to the accumulation and aggregation of the protein in the cytoplasm. Upon oxidative stress, the cytoplasmic FUS accumulates in stress granules, which are possible precursors of aggregates observed in the neurons of patients with FUS - positive ALS or FTD. We reported on the further characterization of FUS co-localisation with transporting in neural tissues of patients for ALS and FTD. We focused on RNA - protein interactions of long RNA repeats, which are associated with ALS and FTD. We have reported the discovery of the interaction between GGGGCC repeat with hnRNPH protein and confirmed this interaction in the nervous tissue of patients, which indicates the importance of the interaction in ALS and FTD.

We have continued with the research aimed at improving the surface display on Lactococcus lactis, as well as some other lactic acid bacteria, with the goal to improve their biotechnological applicability. We have finished and published the results of the study on the improvement of the carrier

protein BmpA, which enabled the covalent attachment of recombinant proteins to the surface of Lactococcus lactis. We improved the surface display of recombinant proteins, bound in a non-covalent manner, with the use of peptidoglycan-binding LysM repeats. The efficacy of such a surface display we tested in ten different species from the genus Lactobacillus and noticed large differences among various species. We have confirmed the relationship

between the efficiency of the surface display and the content of lipoteichoic acid in the bacterial cell wall and demonstrated that the surface display in Lactococcus lactis is improved by limiting the production of lipoteichoic acid.

In collaboration with the Institute of Biotechnology of the ASCR in Prague (Czech Republic) we began the development of specific low-molecular

A member of the department was a recipient of the Zois award for outstanding achievements in the field of proteolytoic enzymes and their regulation. binding molecules based on the albumin-binding domain scaffold and directed against the B subunit of the shiga toxin.

We have developed a new method for the simple detection of biliverdin, heme degradation product, in body-fluid samples. A determination of biliverdin is especially important in veterinary diagnostics. The method is based on the specific interaction of biliverdin with an infrared fluorescent protein. The latter requires biliverdin as a cofactor and exhibits infrared fluorescence only after biliverdin binding. The suggested method has acceptable accuracy and precision and, in contrast to the existing methods, enables the parallel testing of a large number of samples. Additionally, the use of infrared fluorescent protein directly from bacterial lysate makes the method cost effective.

The results of the research work at the Department of Biotechnology in 2013 were published in 39 scientific papers in journals with an impact factor, in 12 book chapters, and in 5 published papers from scientific conferences. The Head of Department, prof. Janko Kos, was a recipient of the Zois award for outstanding achievements on the field of proteolytic enzymes and their regulation, awarded by the Government of the Republic of Slovenia. The



Figure 4: Model of BmpA protein and its shortened variant Bmp1, which has significantly improved ability for surface display on the bacterium Lactococcus lactis.

authors of the book Contemporary Phytotherapy received a prestigious award in the field of promotion and popularisation of science "Prometheus for excellence in scientific communication" for 2013 by The Slovenian Science Foundation. The members of the department were also very active in pedagogical work as lecturers and mentors to students preparing diploma and doctoral theses at the University of Ljubljana, University of Maribor and Jožef Stefan Postgraduate School.

Some outstanding publications in the past year

- Mitchel, J., McGoldrick, P., Vance, C., Hortobagyi, T., Sreedharan, J., Rogelj, B., Tudor, Elizabeth L., Smith, Bradley N., Klasen, C., Miller, Christopher C. J., CoopeR, Jonathan D., Greensmith, L., SHAW, Christopher E.: Overexpression of human wild-type FUS causes progressive motor neuron degeneration in an age- and dosedependent fashion. *Acta Neuropathologica*, 2013, 125, 2, 273–288
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Awards and appointments

1. Janko Kos: Zois Award for the highest scientific achievements in the field of proteolytic enzymes and their regulation, Maribor, the Government of the Republic of Slovenia

Organization of conferences, congresses and meetings

1. Organization of the annual meeting of co-workers of the research program "Pharmaceutical biotechnology: knowledge for health" from the Department of Biotechnology at the Josef Stefan Institute and the Chair of Pharmaceutical Biology at the Faculty of Pharmacy of the University of Ljubljana, Slovenia, 21. 11. 2013

Patent granted

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INTERNATIONAL PROJECTS

 ALSTransfid; Stress TDP43 - Does Stress Induced Reduction of Translation Fidelty Play a Role in ALS/FTLD? Fondation Thierry Latran

Prof. Boris Rogelj

 The Role of Cysteine Proteases and their Inhibitors in Split Anergy of Natural Killer Cells to Tumor Cells Slovenian Research Agency

Prof. Janko Kos

RESEARCH PROGRAM

1. Pharmaceutical Biotechnology: Knowledge for Health Prof. Janko Kos

R&D GRANTS AND CONTRACTS

 Response to Water Stress in Common Bean (Phaseolus vulgaris L.): Proteomic Analysis and QTL Mapping Prof. Janko Kos

VISITORS FROM ABROAD

1. Prof. Jawett Anahid, University of California, Los Angeles, USA, 20.-24. 4. 2013

STAFF

Researchers

- Prof. Kristina Gruden*
 Prof. Janko Kos*, Head
- Prof. Janko Kos^{**}
 Prof. Boris Rogelj
- Prof. Borut Štrukeli

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- 5. Asst. Prof. Aleš Berlec
- 6. Dr. Anja Kovanda
- Dr. Milica Perišić Nanut
 Dr. Jure Pohleven, left 01.10.13
- Dr. jure Ponieven, left 01.10
 Dr. Katja Rebolj
- Dr. Katja Rebolj
 Dr. Jerica Sabotič

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- Dysregulation of TDP-43 Expression in Amyotrophic Lateral Sclerosis and Frontotermoral Lobar Degeneration Prof. Boris Rogelj
- Nitroxoline and Its Nerivatives as New Antitumour Drugs
- Dr. Jerica Sabotič 5. Post-Transcriptional Regulatory Networks in Neurodegenerative Diseases
- Prof. Boris Rogelj6. Inhibitors of Cysteine Carboxypeptidases as Regulators of Autoimmune and Neurodegenerative Processes
- Prof. Janko Kos
 Protein Engineering of Recombinant Probiotic Lactic Acid Bacteria for Treatment of Irritative Bowel Disease
 Prof. Borut Štrukelj

NEW CONTRACTS

 Development and Application of New Methods of Genetic Engineering of Probiotic Lactic Acid Bacteria Labena, d. o. o.

Asst. Prof. Aleš Berlec

11. Dr. Sabina Vatovec

Postgraduates 12. Simona Darovic, B. Sc. 13. Katja Lužar, B. Sc. 14. Maja Štalekar, B. Sc. 15. Simon Žurga, B. Sc. Technical and administrative staff

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- 5. Annette Block, Frédéric Debode, Lutz Grohmann, Julie Hulin, Isabel Taverniers, Linda Kluga, Elodie Barbau-Piednoir, Sylvia Broeders, Ingrid Huber, Marc Bulcke, Petra Heinze, Gilbert Berben, Ulrich Busch, Nancy Roosens, Erik Janssen, Jana Žel, Kristina Gruden, Dany Morisset, "The GMOseek matrix: a decision support tool for optimizing the detection of genetically modified plants", *BMC bioinformatics*, vol. 14, pp. [1-14], 256, 2013.
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DEPARTMENT OF ENVIRONMENTAL **N-**2 SCIENCES

Activities in the Department of Environmental Sciences are diverse and varied as the environment itself. They are multidisciplinary, from different natural sciences to even social sciences, in particular, chemical, physical, geological and biological, which define our environment, society, and human activities. With our research work we want to clarify the relationship between natural processes and human activities, and the influence of these activities on human health and the environment. The scope of our studies, educational and technological aspects of research and development are thematically described in chapters: Environmental analytical chemistry, Biological and geochemical cycles, Environment, nutrition, health, Environmental monitoring, Clean technologies and waste management, Risk and environmental impact assessment. The research summaries and outline of the activities of the research groups and centres within the Department of Environmental Sciences is presented in these chapters.



Environmental analytical chemistry

In the field of the analysis of organic compounds we devoted most of our research to studying the fate of *Prof. Milena Horvat* pharmaceutical and personal care product residues in environmental and wastewater samples, and sediments. Compounds of interest included representative nonsteroidal anti-inflammatory drugs, lipid regulators, hormones, tranquilisers, antidepressants, cytostatics, and industrial compounds that produce an endocrine disrupting effect. To improve the sampling, we developed our own passive-sampling method for selected pharmaceuticals and have applied it to surface and ground waters. Currently, the method is being optimised.

In the area of cytostatic research within the framework of FP7 CytoThreat, we developed a series of analytical procedures for determining 5-fluorouracil, capecitabine, cyclophosphamide, ifosfamide, methotrexate, imatinib, vincristin and etoposide and their commercially available metabolites in waste and environmental water samples. We also investigated their presence in hospital and municipal wastewaters and in receiving surface waters. Through our work we show the presence of detectable quantities of these compounds in wastewaters from hospitals where cancer therapies are being conducted. In addition, fluorouracil was present in wastewater-treatment-plant influent. None of the studied cytostatics were detected in the wastewater-treatment-plant effluent and their receiving waters. We also studied the bio- and photodegradation of fluorouracil, capecitabine, methotrexate, imatinib, vincristin and etoposide and our group is the first to identify several novel transformation products formed during these processes. We also organised an interlaboratory study of the determination of selected cytostatics in surface and waste waters and the statistical evaluation of the results is currently being carried out in collaboration with CSIC, Barcelona, Spain.

In the field of endocrine-disrupting compounds, we researched industrial chemicals and personal care-product ingredients, including bisphenol A, triclosan, parabens and benzophenones. For bisphenol A, triclosan, and parabens we modified an analytical procedure developed for human biomonitoring and applied it to wastewaters. We are currently performing pilot-scale biodegradation studies. We also participated in an interlaboratory round-robin study for the determination of selected pharmaceuticals and hormone disruptors in drinking water. For benzophenones, which are structurally a common denominator for UV filters and selected pharmaceuticals and their transformation products, we developed analytical procedures that allowed us to study aqueous and sediment samples. In addition, we studied the cycling of these compounds in the environment with an emphasis on their photodegradation under natural and simulated sunlight.

The Center for Mass Spectrometry in the O2 department participates in the research and application projects of many research groups at the JSI, Slovenian universities, the National institute of Chemistry, Krka and Lek pharmaceutical companies and other users. For the mass spectrometric measurements of organic compounds we used a high-resolution tandem mass spectrometer Q-Tof Premier, equipped with electrospray ionization source (ESI), which is also coupled with an ultra performance liquid chromatograph (UPLC). This instrument in LC-MS mode was used, for example, for the analysis, occurrence, degradation and transformation of Fluorouracil cytostatic in the environment. The Steroid toxicity and detoxification in fungi were measured with GC-MS. With tandem mass spectrometry MS-MS the structures of phototoxic fagopyrins from buckwheat and the composition of the silver fir (Abies alba) bark extract Abigenol and its antioxidant activity were determined.

The use of stable isotopes was introduced to better understand the Neolitic pottery assemblage from the Mala Triglavca and Resnik sites was analysed to obtain insights into vessel use and husbandry practices. Total lipid extracts



Figure 1: Extreme weather conditions such as flooding, snowfalls and fires have an important influence on environmental processes Floods and NPP Krško, Krško 2012

High snow and transmission lines, Kočevje region 2012/2013

Drought, fires and transmission lines, Primorska region 2013 of the pottery samples were subjected to gas chromatography (GC), gas chromatography-mass spectrometry (GC-MS), gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS) and soft ionisation electrospray mass spectrometric techniques ESI Q-TOF MS and ESI Q-TOF MS/MS. The results show that some vessels were used for cooking ruminant meat, while in other traces of mixed non-ruminant and ruminant meat or plants and animal meat cooking were identified. Some vessels were used for milk processing. With this research we enter into the recent discussion on the occurrence, development and expansion of dairy economies in Europe in early prehistory.

We have also introduced a method for determining the content and isotopic composition of fatty acids in milk and cheese. The method is used for determining the geographical origin and authenticity of milk and milk products.

In the area of radiochemical methods wet digestion procedures for the dissolution of biological samples in the determination of ²¹⁰Po were compared. Classical wet ashing over a gas flame with acids on a long-necked Kjeldahl flask, digestion with acids in an Erlenmeyer flask and microwave digestion in a Teflon vessel at temperatures up to 200 °C were investigated. The results obtained showed that the activity concentrations of ²¹⁰Po found in the samples analysed were comparable for all the procedures used.

In the area of chemical metrology the certification of trace elements in candidate Certified Reference Materials for the EU, JRC, Institute for Reference Materials and measurements (IRMM): (i) Determination of trace elements in Lu-foil and (ii) Determination of Au mass fraction in aluminium matrix ERM-EB530A, ERM-EB530B and ERM-EB530C. It is also important to mention our collaboration in stability studies for CRMs prepared by IRMM (ERM-EC680k, ERM-EC681k, ERM-EC590, ERM-EC591, ERM-EF411 and ERM-CE278k). In addition, a series of CCQM Key Intercomparisons was also organized. Based on the excellent performance a series of CMC (*Calibration Measurement Capability*) claims is also planned in 2014, which will be later entered in the KCDB (*Key Comparisons Data Base*). Furthermore, ordinarily participation in inter-laboratory comparison studies organised by IAEA, ISPRA, WEPAL and other reference laboratories is our mission, as well as their organization.

In the framework of the EMRP project ENV02 dealing with Hg traceability issues in car-exhaust measurements the reactivity and stability of various Hg compounds were investigated to support further research in adsorption mechanisms and analytical methods related to clean technology.

Biological and geochemical cycles

Organic geochemical biomarkers combined with a compound-specific isotopic composition were used to determine the sources and transformation pathways of organic matter in the anoxic eutrophic alpine Lake Bled. The use of compound-specific carbon-isotope analyses of sedimentary lipids in recent anoxic sediments indicated that, despite the fact that the biomarker analysis revealed mostly plankton and terrestrial sources of lipids, an important part of the sedimentary

lipids, especially sterols, should be autochthonous of anaerobic microbial origin. A stable isotope approach was further used to identify the sources of polycyclic aromatic hydrocarbons (PAHs) in sediments. It was found that retene (Re) and perylene (Per) are both mainly of natural origin in Zaka Bay, while in anoxic sediments, the value of δ^{13} C determined at a depth of 12-14 cm in the 1950s indicated that Re was of pyrolytic origin. The stream Solznik drains the partially coniferous Lake Bled watershed, which could be the source of Re in Zaka Bay sediments. The distribution of δ^{13} C values of other individual PAH showed that the PAH input to lake sediments was of pyrolytic origin, likely dominated by coal and wood burning. The influence of PAH originating from vehicular emissions could be seen at the sediment depth corresponding to the period 1953-1961.

We continued the studies of carbon mass balance and carbon cycle on the Slovenian territory. The sources of dissolved inorganic carbon in surface- and groundwater in karstic areas were studied. It was found that approximately the same fractions of biogenic (deriving from the decomposition of organic matter and soil CO_2) and geogenic (deriving from the weathering of carbonate rocks) CO_2 are drained from the area by the rivers. In karstic rivers supersaturated with respect to carbonate, tufa precipitation is one of the efficient mechanisms of carbon fixation; however, in Slovenia, the Krka river is the only large stream with tufa barriers. The precipitation rate of river carbonate was estimated and was found to be critically dependent on the turbulence, temperature and the presence of biofilm at the river bottom, although the degassing of CO_2 into it occurs throughout the year along the entire river course. Our research performed in the Gulf of Trieste confirmed that the Gulf is a sink of CO_2 throughout the year. The river plumes of particulate matter and dissolved nutrients play an important role in carbon cycling by direct inputs of terrigenic carbon, enhancing increased biological activity of the Gulf through the supply of riverine

nutrients. In cooperation with the Velenje Coal Mine, the sources of coalbed gases were determined, based upon regular analyses of composition and stable isotope composition of gases in relation to the geomechanical conditions at the excavation fields Preloge and Pesje.

In the framework of the international project coordinated by the International Atomic Energy Agency, the spatial variability of stable isotope composition of snow cover and its influence on the surface runoff and groundwater were studied, in collaboration with colleagues from other Slovenian (University of Ljubljana, Forestry Institute, Anton Melik Geographical Institute, Environment Agency of Slovenia) and Russian (Lomonosov University, Moscow) research institutions.

In collaboration with Croatian colleagues from Ruder Bošković Institute (Zagreb) and the Institute for Oceanography and Fisheries (Split), geochemical and isotopic analyses were used to study nutrient and contaminant transfer and nutrition sources of filtering organisms along the Adriatic Coast on the case of different cultured and wild populations of mussels and invasive serpulids (*Ficopomatus enigmaticus*).

In the framework of the GMOS project further measurements of Hg in air, precipitation, and water continued. In 2013 the measurements of Hg in air using research aircraft were made in the western part of Slovenia.

From the area of applicative research the potential of the re-use of dredged mud from the Port of Koper in civil applications was investigated together with co-workers from the National Building Institute in Ljubljana.

The partitioning of natural radionuclides in sediments and streams affected by the waste piles of a former uranium mine and mill located at Žirovski vrh, Slovenia, was performed by applying a sequential extraction procedure. The results definitely showed that the total activity concentrations at sites downstream of the influence of the waste piles were higher than at sites upstream of the piles. This difference was geographically very limited to a distance of about 5 km downstream. The fractionation of radionuclides upstream and downstream of the area of influence of the waste piles did not appear to be significantly altered.



DMA before (%) 20 1 2 3 5 6 7 patient

need for the individualization of the therapy and its monitoring. The interpersonal variability of the biotransformation was clearly seen by the excretion of dimethylarsinic acid (DMA) in urine collected daily before the As₂O₃ injection for seven patients.

might be lower than the measured ²²⁶Ra value, which was the case in a core collected from the South Adriatic Pit. Therefore, we proposed a new approach to improve the determination of supported ²¹⁰Pb, which is based on the correction of ²²⁶Ra activity concentrations using the average (²¹⁰Pb/²²⁶Ra) activity ratio in deeper sediment layers. The activity concentrations of ²³⁸U, ²³⁰Th, ²²⁶Ra and ²¹⁰Pb were determined in soil and grass samples collected

from sites at the uranium mill-tailings waste pile. Soil-to-plant transfer factors were determined and the potential use of grass as a monitor of radionuclide migration from the waste pile was evaluated. It was found that grass was not suitable for monitoring ²³⁰Th and ²¹⁰Pb migration, but it has potential in predicting ²³⁸U and ²²⁶Ra migration.

Within the EU 7FP BlackSeaHazNet project, continuous monitoring of radon in soil gas as well as of hydrometeorological parameters were underway. The obtained time-series of data have been analysed using statistical machine-learning techniques (regression-decision trees and artificial neural networks), aimed at studying the influence of tectonic and seismic activities on radon transport mechanisms in soil.

Environment, nutrition, health

Knowing the pharmacokinetics of chemotherapeutics in serum contribute to the optimization of cancer treatment. Conjoint liquid chromatography (CLC) was introduced for the simultaneous two-dimensional separation of ionic forms of metal-based chemotherapeutics from the portions bound to serum proteins. The method is based on assembling CIM Protein G and CIM DEAE disks in a single housing, forming a CLC monolithic column. On the first disk chemotherapeutic bound to immunoglobulin G is separated, while on the second disk the unbound form of the chemotherapeutic is separated from the portion bound to albumin and transferrin. In combination with UV and inductively coupled plasma mass spectrometry (ICP-MS) detection of the kinetics of binding of cisplatin, carboplatin and oxaliplatin to serum proteins was investigated in spiked human serum. The CLC method was introduced to the field of metallomics for the first time.

Selenoproteins and MT mRNA expression were studied in APL patients during arsenic trioxide treatment. The gene expression of six metallothionein (MT) (sub) isoforms, namely MT2a, MT1 (a, e, f, x) and MT3, together with four selenoproteins was followed by qPCR. The weak influence on MTs and suppressed gene expression of selenoproteins were observed after exposure to therapeutic concentrations of arsenic (up to $2 \mu M As$ in blood serum). The results related to MTs are interesting regarding chemoresistance during cancer treatment and as resistance against the toxic effects of metals present in food and water or in the working environment (occupational exposure), while the effects on selenoproteins is important in relation to the treatment efficiency and the side effects of therapy. Simultaneously, methylation of arsenic and selenium excretion were followed.

Monolithic chromatography in combination with ICP-MS and time-of-flight mass spectrometry (Q-TOF-MS) detection was successfully applied in the investigation of nickel speciations in tea infusions. In addition, a study was performed on a determination of the total nickel concentrations in different foodstuffs. These data are important for subjects allergic to nickel, who should avoid foods with elevated nickel concentrations.



Figure 3: Spatial distribution of radon activity concentration in 400 dwellings all over Slovenia in 2013

The enriched isotopic solutions of 50 Cr(VI) and 53 Cr(III) were applied as tracers in the speciation of Cr in environmental and food samples. The data revealed that toxic Cr(VI) cannot exist in foodstuffs of plant origin like tea infusions and bread samples. The isotopic 50 Cr(VI) and 53 Cr(III) solutions were also used to follow the transformation of chromium species (oxidation - reduction) during the extraction of chromium from soil samples and in the optimization of the extraction procedure. Accurate quantification of exchangeable Cr(VI) in soil samples was further performed by the isotope dilution (ID)-ICP-MS technique.

In collaboration with the Catholic University of Louvain the uptake of arsenic in hydroponically grown rice exposed to iron and arsenic was studied. Along rice roots the iron hydroxides precipitate and include arsenic as well as reducing arsenic uptake and toxicity. Together with Swedish scientists the influence of arsenic contaminated rice on the human health of an exposed population in Bengal (India) was evaluated. We also studied the arsenic speciation in the larvae of aquatic insects in pools with high, but localized, arsenic levels along streams in Sweden. The larvae contained high

levels of inorganic arsenic, but fish who feed on them had very low arsenic levels. Most probably the fish live in a much bigger territory than the larvae and feed on mostly uncontaminated larvae from cleaner parts of the stream.

To investigate the impact of Se on Tartary buckwheat (*Fagopyrum tataricum* Gaertn.) plants, the plant foliage was sprayed with 10 mg Se(VI) L^{-1} at the beginning of flowering. The Se was effectively assimilated by the plants and taken into the seeds, where its concentration was more than double that in untreated plants. The seeds were collected and sown to obtain the progeny of these Se-treated plants. To assess the physiological characteristics of control plants and these Se-treated progeny plants, the estimated respiratory potential via electron transport system (ETS) activity and the photochemical efficiency of photosystem II were measured. Three weeks after germination, the Se-treated progeny plants showed higher ETS activity compared to the controls. Through weeks 4 and 5, this high ETS activity approximately halved, and the difference in ETS activity seen at 3 weeks was lost. On the other hand, at week 4, the potential photochemical efficiency was higher in the Se-treated progeny plants than in the controls. In adult plants, the leaves' dry mass was significantly greater in the Se-treated progeny plants than in the controls. This study demonstrates the impact of Se in tartary buckwheat on the progeny plants of Se sprayed plants.

Selenium and selenium species were studied in shellfish in the Slovenian market. In one of the studies we included two main fish species that represent the most commonly consumed fresh fish in Slovenia; trout (*Oncorhynchus mykiss*) and seabass (*Dicentrarchus labrax*) from different locations (Slovenia, Italy, Greece) and environments (fish grown in fish farms and wild fish from their natural environment). Our aim was to compare the differences in selenium and its species amount between fish from farms and fish in their natural environment.

Stable isotope composition $({}^{2}H/{}^{1}H, {}^{3}C/{}^{12}C, {}^{15}N/{}^{4}N, {}^{18}O/{}^{16}O)$, elemental composition and selected physical parameters (fruit mass, antioxidant activity, content of ascorbic acid and total phenols) were used to differentiate Slovenian apples according to their geographical origin. The database on Slovenian milk was established, containing isotopic parameters, elemental and fatty acid composition.

In radon (²²²Rn) research we focused on the air in dwellings, karst caves and soil. A relationship was sought between the concentrations of radon and carbon dioxide in different yearly seasons at different points in the Postojna Cave. Correlation was usually good, with correlation coefficient R² reaching 0.85, except in the closed and feebly ventilated Pisani rov corridor in which levels of both gases were by an order of magnitude higher, showing R²=0.91 in spring and R²=0.61 in summer. This difference has been explained by an additional radon source in summer, when the ventilation is minimal because the outside air temperature is higher than in the cave. In this cave also effect of the nano aerosol concentration and particles size distribution (5–1100 nm range) on the formation of radon short-lived products (²¹⁸Po, ²¹⁴Pb, ²¹⁴Bi and ²¹⁴Po) and their attachment to aerosol particles was investigated.

The aerosol characteristics were influenced by the weather conditions and tourist visits. Our special focus has been product atoms associated with the <50 nm particles, the crucial datum in radon dosimetry.

In a systematic survey, co-funded through a SCOPES project, solid-state nuclear track detectors were exposed twice for half a year, to measure the activity concentrations of radon and thoron (220 Rn) and their short-lived products in one dwelling in each of 400 squares of 7 km × 7 km size covering the entire country. The average annual effective doses will be calculated and the exposure of the general population to radon and thoron will be evaluated. As in previous surveys, the majority of higher levels have been found over carbonate bedrock, and very often that occurred also in new buildings. In a bilateral cooperation with Serbia, complex environmental analyses of indoor air in several selected dwellings in both Slovenia and Serbia have been performed, comprising carbon dioxide, radon and its products (with an emphasis on <50 nm), thoron, nano aersol (number concentration and particle size distribution), and positive and negative ions (< nm).

Within the EU 7FP CITI-SENSE project (Development of sensor-based Citizens' Observatory Community for improving quality of life in cities) pilot study was designed within which air quality will be monitored at selected outdoor locations, as well as indoor in schools and on the participatory principle during movement of people wearing mobile units.

In the frame of the EU 7FP ArcRisk project (Impacts on health in the Arctic and Europe owing to climate-induced changes in contaminant cycling) study on the exposure of European population to mercury was performed. The results of the study were published in the Environmental toxicology and chemistry journal as an review article entitled "Mercury exposure and effects in Europe.

Environmental technologies

In collaboration with BF, University of Ljubljana, we investigated the influence of pharmaceutical diazepam on the structure and phylogenetic composition of the bacterial community in activated sludge from a series of pilot wastewater treatment plants. Based on our findings, only a small proportion of the bacterial consortia are responsible for the increased removal efficiency of diazepam in the bioreactors. The high diversity of bacteria in the reactors with the addition of diazepam indicates that the studied pharmaceutical is nontoxic to the bacteria in activated sludge at the concentration applied ($100 \mu g/L$). We also researched the biodegradation potential of proteobacterial and fungal laccases, i.e., enzymes that have the potential to degrade compounds with aromatic, particularly phenolic structures. Batch biodegradation experiments with laccases Bacillus and ThioLacc indicated their high potential for the biodegradation of bisphenol A, whereas the enzymes were less efficient in degrading ibuprofen, clofibric acid, ketoprofen, diazepam, carbamazepine and diclofenac.

In collaboration with FS and FGG, University of Ljubljana we investigated the potential of cavitation as a wastewater-treatment technology. Hydrodynamic cavitation was for the first time evaluated for the simultaneous removal of clofibric acid, ibuprofen, naproxen, ketoprofen, carbamazepine and diclofenac in complex WW matrices.

In collaboration with the Department of Inorganic Chemistry and Technology we continued our research on cost-effective methodologies for the removal of mercury in flue gasses by an oxidation method in flue-gas desulfurization plants. Mathematical models were introduced and used for the simulation of aqueous Hg chemistry. Mercury behaviour in solid samples at higher temperatures was also studied as part of the initial experiments for the removal of Hg from gases at higher temperatures.

Risk and environmental impact assessment

The most demanding and comprehensive work in 2013 was the Sustainability appraisal of energy policy development of Slovenia by 2030 and beyond as a basis for strategic orientation and decision-making. The focus was on possible further nuclear-energy development. In the framework of consultancy work for GEN energija d.o.o., a revised report on damages caused by Fukushima NPP has been made, while for the industrial partner TKK Srpenica a concept of risk reduction has been provided. Work on international projects covered activities related to the Coordinated Research Project "Techno-economic Evaluation of Options for Adapting Nuclear and Other Energy Infrastructure to Long-term Climate Change and Extreme Weather", which is coordinated by the IAEA.

The radiological risk to wildlife around the former uranium mine and mill located at Žirovski vrh, Slovenia was assessed by the ERICA Tool and found to be negligible. Activity concentrations in bovine milk from the area of Žirovski vrh were comparable to the reference location, except for uranium, where the content was higher. The combined annual effective dose for adults consuming milk from the Žirovski vrh area is $13.0 \pm 1.7 \,\mu$ Sv a⁻¹.

Based on the technical documentation prepared among the others by co-workers from O2, the "Minamata Convention on Mercury" was adopted under the auspices of the UNEP organisation. The Convention is an international treaty designed to protect human health and the environment from anthropogenic emissions and releases of mercury and mercury compounds. Our contribution resulted in two chapters of the report dealing with global releases and the cycling of mercury.

Environmental Monitoring

In collaboration with Chemical Office of the Republic of Slovenia, University Medical centre Ljubljana, regional institutes of Public Health, regional hospitals and health we continued national human biomonitoring. We analyse toxic chemicals including toxic metals (cadmium, lead, mercury) and persistent organic pollutant including dioxins, pesticides, PCBs, polybrominated flame retardant in human blood, urine and maternal milk. Results will be used for the assessment of the burden of the Slovenian population with these environmental pollutants. The regular monitoring programme comprised measurements for updating the database on the isotopic composition of Slovenian wines in accordance with EU regulations, and the isotopic composition of precipitation in Slovenia.

In collaboration with the Environmental Agency of the Republic of Slovenia the monitoring of organotin compounds in surface and sea water was continued in 2012.

The monitoring of natural radionuclides within the influential area of the former uranium mine and mill at Žirovski vrh was performed.

We participated in the Off-Site Monitoring of Krško Nuclear power plant by determining the strontium and tritium in environmental samples. Also, we determined the tritium and C-14 in gas effluents from the nuclear power plant. The used methods are accredited by the Slovenian accreditation body (SA LP-090).

In the Department of Environmental Sciences there is also an active mobile chemical laboratory ELME (ecological laboratory with a mobile unit) organized with four intervention teams that are qualified for the fast and effective action in environmental accidents with hazardous materials, determining the parameters of the field, to assess the impact of pollution on the environment and human health and consultation to the neutralisation of the effects of pollution. The chemical mobile unit had four interventions in 2013 because of chemical accidents and environmental pollution.

Some outstanding achievements

- 1. A method to assign the sources of pollutants such as polycyclic aromatic hydrocarbons (PAH) was developed.
- An analytical method for the determination of fluorouracil in environmental samples that is more sensitive than existing methods was developed.
- In collaboration with the National Institute of Biology, the estrogenicity assay ER-Calux[®] to be able to test raw waste-water samples without the need for sample extraction was developed.
- In collaboration with the Faculty of Mechanical Engineering and the Faculty for Civil Engineering, University
 of Ljubljana, we evaluated the efficiency of hydrodynamic cavitation for removing micropollutants from
 wastewaters.
- 5. For the first time we were able to quantitatively assess the contribution of contaminated sites to the global mercury budget.
- 6. Conjoint liquid chromatography (CLC) was introduced for the simultaneous two-dimensional separation of ionic forms of metal-based chemotherapeutics from the portions bound to serum.

Some outstanding publications in the past year

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- Zupanc, M., Kosjek, T., Petkovšek, M., Dular, M., Kompare, B., Širok, B., Stražar, M., Heath, E.: Shear-induced hydrodynamic cavitation as a tool for pharmaceutical micropollutants removal from urban wastewater. *Ultrasonics Sonochemistry*, 2013, 27

Awards and appointments

 Dr. Tea Zuliani, Prof. Radmila Milačič, Dr. Janez Ščančar: the Poster Prize at the "2013 Winter Conference on Plasma Spectrochemistry" for the presentation "Cr(VI) determination in soil solution by speciated isotope dilution ICP-MS", Krakow, Poland, 10.–15. 2. 2013

Organization of conferences, congresses and meetings

- Milena Horvat: Workshop: Mercury Environment, health and cultural heritage, Ljubljana, Slovenia, 15.–21.
 6. 2013
- 2. Milena Horvat: Training programme for the determination of trace elements in human biological samples, Ljubljana, Slovenia, 9.–19. 12. 2013

INTERNATIONAL PROJECTS

- 1. Determination of the isotopic composition of carbon in sugar samples Prof. Nives Ogrinc
- 2. Analyses
- Prof. Vekoslava Stibilj
- Provision of Testing Services for Filter Media used in IMS Radionuclide Stations The Preparatory Commission For The Comprehensive Prof. Ljudmila Benedik
- Small Services in the Years from 2007 to 2014 Prof. Milena Horvat
- Analyses of Metals, TBT and DBT in Sediments, Mussels and Fish
- Prof. Janez Ščančar
 7FP iNTeg-Risk; Early Recognition, Monitoring and Integrated Management of Emerging, New Technology Related Risks
 - European Commission Prof. Branko Kontić
- 7FP ArcRisk; Arctic Health Risks: Impacts on Health in the Arctic and Europe Owing to Climate-induced Changes in Contaminant Cycling European Commission
- Prof. Milena Horvat
- 7FP GMOS; Global Mercury Observation System European Commission
- Prof. Milena Horvat
- 7FP CYTOTHREAT; Fate and Effects of Cytostatic Pharmaceuticals in the Environment and the Identification of Biomarkers for and Improved Risk Assessment on Environmental Exposure European Commission
 - Prof. Ester Heath
- 7FP BlackSeaHazNet; Complex Research of Euarthquake's Prediction Possibilities, Seismicity and Climate Change Correlations European Commission Prof. Janja Vaupotič
- 7FP CITI-SENSE; Development of Sensor-based Citizens' Observatory Community for Improving Quality of Life in Cities European Commission
 - Prof. Milena Horvat
- 12. 7FP HEALS; Health and Environment-wide Associations Based on Large Population Surveys
 - European Commission Prof. Milena Horvat
- PartEmission; EMRP Emerging Requirements for Measuring Pollutants from Automotive Exhaust Emissions Euramet E.v.
- Prof. Milena Horvat
- EMRP; Traceable Measurements for Monitoring Critical Pollutants under the European Water Framework Directive (WFD-2000/60/EC) Euramet E.v.
 - Euramet E.v. Prof. Radmila Milačič
- 15. LIFE12 ENV/ CROME-LIFE; Cross-Mediterranean Environment and Health Network European Commission
- Prof. Milena Horvat 16. Stable Isotope Technique to Assess Human Milk Intake in Infants Living in Areas Contaminated with Mercury, Lead and Cadmium; Stable Isotope Technique to Assess Human Milk Intake in Infants Living in Contaminated Areas IAEA - International Atomic Energy Agency Prof. Milena Horvat
- 17. Use of Environmental Isotopes in Investigations of Influence of Snow Melt on Stream Runoff in the Area of Julian Alps, NW Slovenia IAEA - International Atomic Energy Agency Dr. Polona Vreča

- Assessment of Human Milk Intake in Infants Living in Gold Mining Areas in South West Nigeria, Using Stable Isotope Techniques IAEA - International Atomic Energy Agency
 - Dr. Darja Mazej
- Training in Radiochemistry and Radioactivity Measurements for Practitioners from Countries Eligible under the JRC Enlargement & Integration Policy Institute For Reference Materials And Measurements Prof. Ljudmila Benedik
- Training Fee for Ms Christiane Odumah Anderson, (Ghana), 1.10. 24. 12. 2012, 8.9.-7.12.2013
 Ictp - Centro Internazionale Di Fisica Teorica
 - Prof. Milena Horvat
- SOP WHO Standard Operating Procedure World Health Organization Prof. Milena Horvat
- Determination of Ag in Chicken Paste and Ag Suspension by k0-INAA Institute For Reference Materials And Measurements Dr. Radoiko Iaćimović
- Determination of Ag in Ag Suspension by k0-INAA Institute For Reference Materials And Measurements Dr. Radojko Jaćimović
- 24. Techno-economic Evaluation of Options for Adapting Nuclear and Other Energy Infrastructure to Long-term Climate Change and Extreme Weather IAEA - International Atomic Energy Agency Prof. Branko Kontić
- Determination of Total Na and Cl in Ion Exchange Resins by K0-INAA University Of Pavia (lena)
 Dr. Radojko Jaćimović
- Radojko Jachnović
 Determination of Trace Elements in Lu Foil by k0-INAA and XRF Institute For Reference Materials And Measurements Dr. Radojko Jaćimović
- Radoko Jacimoric
 Stability Study of ERM-EC680k and ERM-EC681k Institute For Reference Materials And Measurements Dr. Radojko Jaćimović
- IAEA Fellowships for Mr Baktyiar Zholboldiev, Ms Asel Seitkazieva and Mr Asankul Nurabaev, KIG/13006, KIG/13012, KIG/13013, 22.04.2013 - 21.06.2013
 IAEA - International Atomic Energy Agency Prof. Ljudmila Benedik
- Training Fee for Ms Ilona Matveyeva, (Kazakhstan), 1.6.-29.8.2013 Ictp - Centro Internazionale Di Fisica Teorica Prof. Milena Horvat
- The Stability Study for Br in ERM-EC590 and ERM-EC591 by k0-INAA Institute For Reference Materials And Measurements Dr. Radojko Jaćimović
- Stability Study of ERM-CE278k by CVAAS, ICP-MS and k0-INAA Institute For Reference Materials And Measurements Dr. Radoiko Iaćimović
- IAEA Fellowship for Mr Dejan Jani, MNE/12007, 2.9.-1.11.2013; Analysis and Speciation of Trace Elements by ICP MS and Similar Techniques IAEA - International Atomic Energy Agency Prof Milena Horvat
- 33. The Stability Study for Co, Sb, Se, V and Zn in Coal Materials; Stability Study of ERM-EF411 by k0-INAA Institute For Reference Materials And Measurements
- Dr. Radojko Jaćimović 34. 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...

IÁEA - International Atomic Energy Agency

Prof. Nives Ogrinc



- Stability Study of ERM-EC590 and ERM-EC591 by k0-INAA Institute For Reference Materials And Measurements Dr. Radojko Jaćimović
- 36. Stability Monitoring of ERM-CE477; Measurements of Monobutyltin (MBT), Dibutyltin (DBT) and Tributyltin (TBT) in the Reference Material ERM-CE477 Institute For Reference Materials And Measurements Dr. Tea Zuliani
- IAEA Fellowship for Ms Snežana Anđelić, MNE/12008, 11.11.-10.12.2013 IAEA - International Atomic Energy Agency Prof. Milena Horvat
- Determination of Au in Al-Au Alloy by INAA Institute For Reference Materials And Measurements Dr. Radojko Jaćimović
- Mercury Analysis and Speciation in the Oceans Javna agencija za raziskovalno dejavnost RS Prof. Milena Horvat
- 40. Fluid Dynamics and Carbon Cycling in Sedimentary Basins: Geochemical Characterization, Evaluation of Biogeochemical Processes and Modeling Javna agencija za raziskovalno dejavnost RS Dr. Tjaša Kanduč
- Calibration of Palaeoenvironmental Records in (Sub)recent Laminated Tufa Javna agencija za raziskovalno dejavnost RS Prof. Sonja Lojen
- Determination of Toxicity and Physico-chemical Properties of Pharmaceuticals Javna agencija za raziskovalno dejavnost RS Dr. Tina Kosjek
- Ana Rosek
 Tracing of Natural and Anthropogenic Impacts in Marine Ecosystem Along Istrian Adriatic Coast Using Mediterranean Mussel M. Galloprovincialis Javna agencija za raziskovalno dejavnost RS
- Dr. Tjaša Kanduč
 44. Environmental Isotopes in Snow Hydrology
- Javna agencija za raziskovalno dejavnost RS Dr. Polona Vreča
- 45. Mercury Processes in Aquatic Systems; Mercury Methylation and Reduction in Natural Aquatic Environments: Laboratory Studies using High Specific Activity 197Hg Radiotracer Javna agencija za raziskovalno dejavnost RS Prof. Milena Horvat
- 46. Where Radon (Gaseous Soil Component) is coming from? Javna agencija za raziskovalno dejavnost RS Prof. Janja Vaupotič
- Evaluating the Vulnerability of Groundwater Resources using Groundwater Tracers Javna agencija za raziskovalno dejavnost RS
- Prof. Nives Ogrinc 48 The Impact of Colloidal Particles on t
- 48. The Impact of Colloidal Particles on the Fate of Trace Elements in Environmental Compartments

Javna agencija za raziskovalno dejavnost RS Prof. Radmila Milačič

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. Tartary buckwheat as a new source for functional foods Prof. Vekoslava Stibilj
- Synthesis, characterisation and use of novel ruthenium compounds in electrochemotherapy of tumors (basic research project) Prof. Janez Ščančar
- Sustainable land use in relation to soil and crop quality Prof. Nives Ogrinc
- Metagenomics for bioexploration and biomining of bacterial laccases for a sustainable environment Prof. Ester Heath
- Archaeologies of hunter-gatherers, farmers and metallurgists: Cultures, populations, palaeoeconomies and climate
- Prof. Nives Ogrinc6. Advanced water treatment with ultrasound and cavitation Prof. Ester Heath
- Toxic metals and organometallic compounds in the terrestrial environment Prof. Radmila Milačič
- 8. Speciation and interactions of chemical contaminants at trace level in aqueous media

- to support the developement of cost-effective removal technologies Prof. Milena Horvat
- 9. The effect of iodine and selenium on growth and quality of crops Prof. Vekoslava Stibilj
- Groundwater age determination in deep aquifers of Slovenia Prof. Sonja Lojen
- Sediments in aquatic environments: their geochemical and mineralogical characterization, remediation, and use as secondary raw materials Prof. Radmila Milačič
- Petrology of brown (low-rank) coals as mined and/or used in Slovenia, natural gasses in them, and their gas-sorption properties Dr. Tjaša Kanduč
- 13. Carbon dynamics in forest soils and the rhizosphere Prof. Nives Ogrinc
- Optimization and validation of new indicator systems in complex environmental matrices
- Prof. Milena Horvat15. Evaluating geological sequestration of CO2 in low rank coals; Velenje basin, Slovenia as a natural analogue
- Dr. Tjaša Kanduč
- Pharmaceutical and personal care product residues in the environment: Occurence, sources, treatment and effects
- Prof. Ester Heath 17. Farming Possibilities in Water Protection Areas
- Prof. Sonja Lojen 18. Farming Possibilities in Water Protection Areas
- Prof. Sonja Lojen 19. The use of specific methods for determination and prevention of adulteration of milk
- The use of specific methods for determination and prevention of adulteration of milk and dairy products Prof. Nives Ogrinc
- The use of specific methods for determination and prevention of adulteration of milk and dairy products Prof. Nives Ogrinc
- Quality of fish on Slovenian market and analysis of possibilities to adjust supply to demand with respect to secure nutritional safety and increase competitiveness of fisheries and aquaculture(Healthy fish - healthy as fish: competitive fisherm Prof. Vekoslava Stibilj
- 22. Quality of fish on Slovenian market and analysis of possibilities to adjust supply to demand with respect to secure nutritional safety and increase competitiveness of fisheries and aquaculture(Healthy fish - healthy as fish: competitive fisherm Prof. Vekoslava Stibili
- EMRP PartEmission, Emerging Requirements for Measuring Pollutants from Automotive Exhaust Emissions Prof. Milena Horvat
- EMRP; Traceable Measurements for Monitoring Critical Pollutants under the European Water Framework Directive (WFD-2000/60/EC)
- Prof. Radmila Milačič 25. Analyses of Carbon and Oxygen
- Dr. Polona Vreča
- Chinese-Norwegian-Slovenian Workshop: "Mercury, Environment, Health and Cultural Heritage", 15-21 June 2013, Ljubljana, Slovenia Prof. Milena Horvat
- Determination of Elements in Environmental Samples by Neutron-activation Method using TRIGA Mark II Reactor Prof. Borut Smodiš

NEW CONTRACTS

 Evaluating gelogical sequestration of CO2 in low rank coals; Velenje basin, Slovenia as a natural analogue Premogovnik Velenje, d. d.

Premogovník Velenje, d. d Dr. Tjaša Kanduč

- Sustainability appraisal of energy policy development in Slovenia by 2030 with the emphasis on nuclear option.
 - Gen Energija, d. o. o. Prof Branko Kontić
- Branko Konde
 Human biomonitoring in Zasavje chemical analyses Ministrstvo za Zdravje Republike Slovenije
- Ministrstvo za Zdravje Republike Slovenije Prof. Milena Horvat
- 4. Co-financing of activities of holder of national standard in 2013 amount of substance / soil

Ministrstvo za Gospodarski Razvoj in Tehnologijo Dr. Polona Vreča

- Consultancy on environmental impact evaluations related to planned NPP2 Krško GEN energija, d.o.o. Prof. Branko Kontić
- Optimization and validation of new indicator systems in complexenvironmntal matrices

Inštitut za mikrobiološke znanosti Prof Milena Horvat

Pharmaceutical and personal care product residues in the environment: Occurrence, sources, treatment and effects Institut za ekološki inženiring d.o.o. Prof. Ester Heath

VISITORS FROM ABROAD

- Dr. Bojan Hamer, Emina Durmiši, Ruđer Bošković Institute, Center for Marine Research, 1. Zagreb, Croatia, 18.-19. 1. 2013
- Adrian Vicent Claramunt, Leonardo da Vinci Fellowship, Valencia, Spain, 25. 1.-23. 5. 2013 2
- Michal Buch, University of Wrocław, Wrocław, Poland, 20. 2. 2013
- Dávid Horváth, Institute of Radiochemistry and Radioecology, University of Pannonia, 4. Vészprem, Hungary, 1. 3.-31. 5. 2013
- 5 Baktyiar Zholboldiev, Asel Seitkazieva, Asankul Nurabaev, Ministry of Emergency Situation of the Kyrgyz Republic, Agency for Managing Tailing under the Ministry of Emergency Situations of the Kyrgyz Republic, The Kyrgyz Republic. Biology and Soil Institute of the National Academy of Science KR, Laboratory Biogeo, Bishkek, Kyrgyz, 21. 4.-30. 6. 2013
- 6. Dr. Maria Angela Menezes, CDTN/CNEN, Belo Horizonte, Brazil, 14.-26. 5. 2013
- Dr. Jennifer C. McIntosh, University of Arizona, Tucson, USA, 16.-24. 5. 2013
- 8. Ilona Matveyeva, Al-Farabi Kazakh National University, Almaty, Kazakhstan, 1.6.-29.8.2013
- Mariam Todadze, Institute of Geophysics, Ivane Javakhishvili Tbilisi State University, 9. Tbilisi, Georgia, 10.-25. 6. 2013
- 10. Tang Dingding, Liu Ning, Xia Yingxian, Fang Li, Wu Jianmin, Wang Zuguang, Ministry of Environmental Protection, Beijing, China, 15.-21. 6. 2013
- 11. Prof. Duan Lei, School of Environment, Tsinghua University, Beijing, China, 15.-21. 6. 2013 12. Prof. Feng Xinbin, Prof. Qiu, Guangle, Institute of Geochemistry, Chinese Academy of
- Sciences, Guiyang, China, 15.-21. 6. 2013 13. Dr. Thorjørn Larssen, Dr. Yan Lin, Norwegian Institute for Water Research, Oslo,
- Norway, 15.-21. 6. 2013 14. Volodymyr Vashchenko, Ministry of Ecology and Natural Resources of Ukraine, Kiev,
- Ukraine, 12. 8. 2013
- 15. Olena Vashchenko, National Pedagogical Dragomanov University, Kiev, Ukraine, 12.8.2013
- 16. Dr. Dejan Jančić, PI Center for Ecotoxicological Research of Montenegro, Podgorica, Montenegro, 1. 9.-1. 11. 2013
- 17. Dr. Vladimir P. Smolyar, Department of Theoretical and Experimental Nuclear Physics, Odessa National Polytechnic University, Odessa, Ukraine, 3. 9.-4. 10. 2013
- 18. Prof. Ryoko Fujiyoshi, Faculty of Engineering, Hokkaido University, Sapporo, Japan, 10.-20.9.2013

STAFF

Researchers

- Prof. Ljudmila Benedik 1.
- Asst. Prof. Ingrid Falnoga 2
- 3. Prof. Ester Heath
- Prof. Milena Horvat, Head 4.
- Dr. Radojko Jaćimović
- Asst. Prof. Zvonka Jeran 6.
- Dr. David Kocman 7.
- 8. Prof. Branko Kontić
- 9. Dr. Tina Kosjek
- 10. Dr. Jože Kotnik
- Asst. Prof. Sonja Lojen 11.
- 12. Prof. Radmila Milačič
- 13. Prof. Nives Ogrinc 14. Prof. Borut Smodiš
- 15. Prof. Vekoslava Stibilj
- 16. Prof. Janez Ščančar
- Asst. Prof. Zdenka Šlejkovec 17.
- 18. Prof. Janja Vaupotič
- 19. Dr. Polona Vreča
- 20. Dr. Tea Zuliani
- 21. Dr. Dušan Žigon
- Postdoctoral associates
- 22. Dr. Urška Dermol, left 01.04.13
- 23. Dr. Tjaša Kanduč
- 24. Dr. Davor Kontić
- 25. Dr. Darja Mazej
- 26. Dr. Ana Miklavčič Višnjevec
- 27. Dr. Marko Štrok
- 28. Dr. Mitja Vahčič, left 01.03.13

- Pharmaceutical and personal care product residues in the environment: Occurrence, 8 sources, treatment and effects JP CČN Domžale-Kamnik d.o.o. Prof Ester Heath
- Dr. Oleksandr Lyashchuk, National Antarctic Scientific Centre, Kiev, 21. 9.-25. 10. 2013 19.
- 20. Dr. Volodymyr Bakhmutov, Institute of Geophysics, National Academy of Sciences of Ukraine, Kiev, Ukraine, 21. 9.-25. 10. 2013
- 21. Dr. Sergio Ribeiro Guevara, Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Bariloche, Argentina, 15. 9.-13. 10. 2013
- 22. Dr. John Bennett, The Australian Nuclear Science and Technology Organisation (ANSTO), Lucas Heights NSW, Australia, 27.-30. 9. 2013
- 23. Christiana Odumah Anderson, Department of Physics, University of Cape Coast, Cape Coast, Ghana, 9. 10.-7. 12. 2013
- 24. Dr. Neven Cukrov, Ruđer Bošković Institute, Zagreb, Croatia, 23. 10. 2013
- 25. Nuša Cukrov, Ruđer Bošković Institute, Zagreb, Croatia 4.-30. 11. 2013
- 26. Dr. George Melikadze, Mariam Todadze, Institute of Geophysics, Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia, 14.–28. 11. 2013
- 27. Nikolay Kiyashko, General and Inorganic Chemistry Department, Al-Farabi Kazakh National University, Almaty, Kazakhstan 4.–11. 12. 2013
- 28. Nino Kapanadze, Vladimer Chikviladze, Institute of Geophysics, Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia, 8.–24. 12. 2013
- 29. Dr. Zora S. Žunić, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, 15.-22. 12. 2013
- 30. Dr. Predrag Kolarž, Institut za fiziku, Belgrade, Serbia, 15.-22. 12. 2013
- 31. Elizaveta Mochalova, Geological Institute of the Russian Academy of Sciences, Moscow, Russia, 9.-19. 12. 2013
- 32. Konstantin Ossipov, Lomonosov Moscow State University, Moscow, Russia, 9.-19. 12. 2013
- 33. Dalė Baranauskienė, Vaida Bakšenskaitė, Lithuanian University of Health Sciences Neuroscience Institute, Kaunas, Lithuania, 9.–19. 12. 2013
- 34. Biljana Manevska, Department of reference laboratories Trace elements analysis laboratory, Institute of Public Health of R. Macedonia, Skopje, Macedonia, 9.-19. 12. 2013
- 35. Nataša Janev Holcer, Croatian National Institute of Public Health, Zagreb, Croatia,

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- 9.-19.12.2013 36. Snežana Andelić, Center for Ecotoxicological Research of Montenegro, Podgorica,
- Montenegro, 11 11.-10 12. 2013 Dr. Giulio Cozzi, Fabio P. Polo, Ca' Foscari University, Venice, Italy, 20. 12. 2013
- 38. Prof. Gaetane Lespes, University of Pau, France, 23.-27. 12. 2013

Postgraduates

- 29. Ermira Begu, B. Sc.
- 30. Dr. Mateja Bezek, left 01.04.13
- 31. Dr. Arne Bratkič
- 32. Marko Černe, B. Sc., left 24.10.13
- 33. Marjeta Česen, B. Sc.
- 34. Dr. Marinka Gams Petrišič, left 01.07.13
- 35. Dr. Asta Gregorič, left 01.04.13
- 36. Ana Jerše, B. Sc.
- 37. Urška Kristan, B. Sc.
- 38. Anže Martinčič, B. Sc.
- 39. Petra Novak, B. Sc.
- 40. Breda Novotnik, B. Sc.
- 41. Dr. Tina Oblak, left 01.04.13 42. Majda Pavlin, B. Sc.
- 43. Kelly Peeters, B. Sc.
- 44. Petra Planinšek, B. Sc
- 45. Janja Snoj Tratnik, B. Sc.
- 46 Samo Tamše B Sc
- Janja Vidmar, B. Sc.
 Saša Zavadlav, B. Sc., left 01.04.13
- Technical officer
- 49. Sonja Zagorc, B. Sc.
- Technical and administrative staff
- 50. Vesna Faion
- 51. Damjana Nikovski, B. Sc.

54. Barbara Svetek, B. Sc.

55. Zdenka Trkov, B. Sc. 56. Stojan Žigon

52. Silva Perko, B. Sc 53. Janja Smrke

Annual Report 2013

BIBLIOGRAPHY

ORIGINAL ARTICLE

- 1. Miha Avberšek, Bojana Žegura, Metka Filipič, Nataša Uranjek Ževart, Ester Heath, "Determination of estrogenic potential in waste water without sample extraction", *J. hazard. mater.*, vol. 260, pp. 527-533, 2013.
- Martine Bellanger *et al.* (33 authors), "Economic benefits of methylmercury exposure control in Europe:: Monetary value of neurotoxicity prevention", *Environmental health*, no. 3, vol. 12, 20 pp., 2013.
- 3. Ljudmila Benedik, "An overview of results obtained in intercomparison exercises for determination of actinides", In: Proceedings of the 6th International Conference on Radionuclide Metrology - Low Level Radioactivity Measurement Techniques, 17-21 September 2013, Jeju Island, Korea, *Appl. Radiat. Isot.*, vol. 81, pp. 10-13, 2013.
- 4. Mateja Bezek, Asta Gregorič, Janja Vaupotič, "Radon decay products and 10-1100 nm aerosol particles in Postojna Cave", *Nat. hazards earth syst. sci.*, vol. 13, no. 3, pp. 823-831, 2013.
- Tanja Blagus, Boštjan Markelc, Maja Čemažar, Tina Kosjek, Véronique Préat, Damijan Miklavčič, Gregor Serša, "In vivo real time monitoring system of electroporation mediated control of transdermal and topical drug delivery", *J. control. release*, vol. 172, iss. 3, pp. 862-871, Dec. 2013.
- drug delivery", *J. control. release*, vol. 172, iss. 3, pp. 862-871, Dec. 2013. 6. Arne Bratkič, Nives Ogrinc, Jože Kotnik, Jadran Faganeli, Dušan Žagar, Shinichiro Yano, Akihide Tada, Milena Horvat, "Mercury speciation driven by seasonal changes in a contaminated estuarine environment", In: International Workshop on Mercury in contaminated sites: characterization, impacts and remediation, 10-14 October, 2010, Piran, Slovenia, *Environ. Res.*, vol. 125, pp. 171-178, 2013.
- Mihael Budja, Nives Ogrinc, Andreja Žibrat Gašparič, Doris Potočnik, Dušan Žigon, Dimitrij Mlekuž, "Transition to farming - transition to milk culture: a case study from Mala Triglavca, Slovenia", *Doc. Praehistor.*, 40, pp. 97-117, 2013.
- Manuel Carmona, Wiilias Llanos, Pablo Leon Higueras, David Kocman, "Mercury emissions in equilibrium: a novel approach for the quantification of mercury emissions from contaminated soils", *Analytical methods*, vol. 5, issue 11, pp. 2793-2801, 2013.
- M. Cinta Osácar, Concha Arenas, Marta Vázquez-Urbez, Carlos Sancho, Luis Auqué, Gonzalo Pardo, Sonja Lojen, Neven Cukrov, "Seasonal and decadal stable isotope evolution recorded by recent tufa deposited on artificial substrates in the Monasterio de Piedra Natural Park", *Geogaceta*, vol. 54, pp. 135-138, 2013.
- Neven Cukrov, V. Čuculić, Delko Barišić, Sonja Lojen, L. Mikelić, V. Oreščanin, Neda Vdović, Ž. Fiket, Branko Čermelj, Marina Mlakar, "Elemental and isotopic records in recent fluvio-lacustrine sediments in karstic river Krka, Croatia", *J. geochem. explor.*, vol. 134, pp. 51-60, 2013.
- 11. Damjana Cvelbar, Vanja Žist, Katja Kobal, Dušan Žigon, Marija Žakelj-Mavrič, "Steroid toxicity and detoxification in fungi", In: Special issue of the 16th International Workshop on Molecular Biology of Carbonyl Metabolis, July 10-14, 2012, Plön, Germany, *Chem.-Biol. Interact.*, vol. 202, no. 1/3, pp. 243-258, 2013.
- 12. L. Deroma, Maria Parpinel, Veronika Tognin, L. Channoufi, Janja Snoj Tratnik, Milena Horvat, Francesca Valent, Fabio Barbone, "Neuropsychological assessment at school-age and prenatal low-level exposure to mercury through fish consumption in an Italian birth cohort living near a contaminated site", *Int. j. hyg. environ. health*, vol. 216, issue 4, pp. 486-493, 2013.
- 13. Ryoko Fujiyoshi, Masanori Okabayashi, Yosuke Sakuta, Kazumasa Okamoto, Takashi Sumiyoshi, Ivan Kobal, Janja Vaupotič, "Soil radon in winter months under snowpack in Hokkaido, Japan", *Environmental earth sciences*, vol. 70, issue 3, pp. 1159-1167, 2013.
- 14. Marinka Gams Petrišič, Gregor Muri, Nives Ogrinc, "Source identification of polycyclic aromatic hydrocarbons in Lake Bled (NW Slovenia) sediments using stable carbon isotopes", *Environ. sci. technol.*, vol. 47, issue 3, pp. 1280-1286, 2013.
- 15. Marinka Gams Petrišič, Nives Ogrinc, "Lipid biomarkers of suspended particulate organic matter in Lake Bled (NW Slovenia)", *Geomicrobiol. j.*, vol. 30, issue 4, pp. 291-301, 2013.
- 16. Mateja Germ, Paula Pongrac, Marjana Regvar, Katarina Vogel-Mikuš, Vekoslava Stibilj, Radojko Jaćimović, Ivan Kreft, "Impact of double Zn and Se biofortification of wheat plants on the element concentrations in the grain", *Plant, soil and environment*, vol. 59, no. 7, pp. 316-321, 2013.

- 17. Denis Glavič-Cindro, Ljudmila Benedik, Jasmina Kožar Logar, Branko Vodenik, Benjamin Zorko, "Detection of Fukushima plume within regular Slovenian environmental radioactivity surveillance", In: Proceedings of the 6th International Conference on Radionuclide Metrology Low Level Radioactivity Measurement Techniques, 17-21 September 2013, Jeju Island, Korea, *Appl. Radiat. Isot.*, vol. 81, pp. 374-378, 2013.
- 18. Asta Gregorič, Janja Vaupotič, Franci Gabrovšek, "Reasons for large fluctuation of radon and CO₂ levels in a dead-end passage of a karst cave (Postojna Cave, Slovenia)", *Nat. hazards earth syst. sci.*, vol. 13, no. 2, pp. 287-297, 2013.
- Asta Gregorič, Janja Vaupotič, Kardos Richárd, Mária Horváth, Tibor Bujtor, Tibor Kovács, "Radon emanation of soils from different lithological units", *Carpatian journal of earth and enviroinmental sciences*, vol. 8, no. 2, pp. 185-190, 2013.
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MENTORING

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DEPARTMENT OF AUTOMATION, **BIOCYBERNETICS AND ROBOTICS E-1**

The research strategy within our department is unique, as it supports a variety of multi- and interdisciplinary research projects. Specifically, our research combines the fields of automatics, robotics (including intelligent control, humanoids, cognitive robotics, and robot vision), biocybernetics, kinesiology, ergonomics and environmental physiology. The common theme in all our research endeavours to date has been optimising "the behaviour of man and machine", accounting for interactions with the environment. This past year we have added "human-robot partnership" as an additional goal of our research programme. By combining engineering sciences and life sciences, we have been able to make significant contributions to the development of: new methods for sensorimotor learning by imitation and coaching, a planetary habitat simulation facility, humanoid vision systems, manikins enabling the evaluation of protective garments for industry and recreation, kinematic models of the human body that serve as a basis for the design of anthropomorphic systems, and a medical treatment for frostbite.



The department maintains the Programme Group "Automatics, robotics and biocybernetics" in the Head: field of Production Technology. The Programme group has three major overlapping research foci: Asst. Prof. Leon Žlajpah automation and intelligent control (leader: doc. dr. Leon Žlajpah), humanoid and cognitive robotics (leader: dr. Aleš Ude), and biocybernetics: environmental physiology & ergonomics (leader: prof. dr. Igor B. Mekjavic). By maintaining a critical mass of researchers in all three areas within one Programme group, we have managed to foster exciting multidisciplinary projects.

During the past year, the main research topics in the department included humanoid robotics, the control of robot systems and learning strategies, studies of human physiology in extreme environments, an evaluation of protective equipment, the development of biomedical methods, and the automation of industrial manufacturing.

I. Automation and Intelligent Control

The research orientation within this group is primarily in the development of advanced control strategies for robot systems working in unstructured environments, bio-inspired control systems, cooperating robot systems, the control of multi-arm robots, and the automation of industrial processes. Historical note: Since its inception the department has maintained an inter - and multidisciplinary research focus. The scientific inheritance of its founders includes pioneering research culminating in the first demonstration of how functional electrical stimulation can assist paraplegics to walk, and the development of the first industrial robots in our region. In addition to kinematics, the common denominator in the biomedical and robotic research is improving the quality of life.

Automation, robotics and factory information systems for manufacturing

In 2013 we implemented an automatic cell for a glassblowing operation and integrated it in regular production. The specific target environment is dedicated to the production of several hundred glass items; however, up to now it was predominantly manual. In addition, the technology of main manual operations execution was not

formalized, but in a form of collective experience and skills of the human operators involved. We automated the key manual operation, which only a couple of skilled operators could perform satisfactorily.

Following the applied research and development activities, we implemented the automated solution, which has two aspects. The first part is a system for the construction of formal operation instructions based on the measurement and processing of skilled workers' actions. The second part is the automated cell that, based on the determined formal representations, carries out the glass item production operation. During work, the automated system adapts to parameter changes. It enables the inclusion of new glass objects.



Figure 1: System installation in a manufacturing cell and the training of operators

Advanced robot control

For tasks where more than one robot arm is cooperating the coordinated control becomes rather complex and the control algorithms are time demanding. Therefore, we propose to treat the two-arm or multi-arm robot systems as a single uniform system. This enables us a more efficient and simpler approach to develop control systems for cooperating robots. The advantages are especially noticeable when for the task execution the absolute position/

For the implementation of the applied R&D results, in 2013 we have received two awards:

- Golden award for innovation, Chamber of Commerce and Industry of Slovenia.
- Golden award for innovation, Zasavje
- Regional Chamber of Commerce and Industry.

orientation of the robot end-effectors is not important but rather the relative position/orientation, or when the robot base is moving, e.g., mounted on a mobile platform. Our research focus was two-arm mechanisms. We have developed a method for the modelling of a combined robot mechanism, where the model of the complete system is generated by combining already known models of a particular robot mechanism. Additionally, we have included the task the robot has to perform as a part of the complete model of the robot systems. The task is represented as a virtual mechanism and the task execution is controlled by controlling the motion of this virtual mechanism. By

treating the multi-arm robot system as a uniform system the self-motion, i.e., the redundancy, of the whole system can be exploited more easily, which is visible, especially when avoiding contacts with objects in the robot workspace.

Human in the loop

We developed methods to transfer human motor skills to the robots. These methods are based on including the human cognitive and sensorimotor capabilities into the robot control loop. By operating the robot, the human acquired the skill to perform tasks with the robot. The skill is then extracted/modelled using machine-learning tools and used for autonomous robot operation. The methods were validated on an industrial robot arm and a humanoid robot.

We utilized a special haptic interface to enclose the human tutor in the robot control loop. This interface provided the tutor with the feedback about the state of the humanoid robot upon which the human could react and move

We are using human cognitive and sensorimotor capabilities to teach the robot complex tasks that also require the variable compliance of the robot arm. state of the humanoid robot upon which the human could react and move the robot body joints with the motion of their own body joints. The method for providing the feedback that we proposed is using information about the motion of the robot centre-of-mass and converts it into the forces that act on the human centre-of-mass. We used this method to teach the humanoid robot how to compliantly interact with the human partner.

Moreover, we developed a method for the multi-modal control and teaching of the robots. The robot motion was controlled by the tutor's arm motion measured by the motion capture system. Besides controlling and teaching the robot about the motion we also controlled and taught the robot how to modulate its stiffness by using electro-myography (EMG). By allowing the robot arm to regulate its stiffness, we were able to teach the robot to perform dynamic tasks that involve interactions with an unstructured environment.

Whole-body Compliant Dynamical Contacts for Humanoid Robotics

We studied how humans utilize supportive hand contacts to counteract various postural perturbations. By emulating situations when the balance of an individual was challenged, we examined the functional role of sup-



Figure 2: A method for teaching robots to cooperate with humans in dynamic manipulation tasks.

portive hand contact at different locations where the balance of an individual was perturbed by translational perturbations of the support surface. The effect of the handle position was significant for the perturbations in the posterior direction where the lowest maximum forces were recorded in the handle located at shoulder height. They were comparable to the forces in the handle at eye level and significantly lower than the forces in the handle located either lower or further away from the shoulder. Our results indicate that although the location of a supportive hand contact has no effect on the peak centre-of-pressure displacement of healthy individuals, it affects the forces that an individual needs to exert on the handle in order to counteract support perturbations.

The work was carried out in the scope of the FP7 project Codyco (http:// www.codyco.eu) that aims to advance the current control and cognitive understanding of robust, goal-directed, whole-body, motion interaction with multiple contacts. The project goes beyond traditional approaches by proposing methodologies for performing coordinated interaction tasks with

complex systems; by combining planning and compliance to deal with predictable and unpredictable events and contacts; and by validating theoretical advances in real-world interaction scenarios.

II. Humanoid and Cognitive Robotics Lab

The aim of the research Humanoid and Cognitive Robotics Lab is to create robots capable of helping people and interacting with them in natural environments. Since humanoids are similar to humans, it is much easier for people to interact with humanoids than with other types of robots. We therefore believe that cognitive humanoid robots are the key to the development of robot companions that can help people in their homes, which is one of the most important challenges for robotics research.

The Humanoid and Cognitive Robotics Lab is involved in a number of EU projects from the program "Cognitive Systems and Robotics". Most of our work in 2013 was performed within the program group "Automation, robotics and biocybernetics", and the FP-7 projects Xperience, IntellAct, and ACAT:



Figure 3: Two-arm robot holding a plate and avoiding the human moving into the robot's workspace.

large-scale integrated project "Robots bootstrapped through learning from experience" (Xperience), which has 7 partners.

STREP project "Intelligent observation and execution of actions and manipulations" (ItellAct) with 6 partners. STREP project "Learning and execution of action categories" (ACAT) with 6 partners. A more detailed description of these projects follows below.

Xperience (http://www.xperience.org/)

Current artificial cognitive systems are limited with respect to the generative mechanisms which rely on prior knowledge are employed to predict the immediate future and are key in increasing the bandwidth and speed of cognitive development. The goal of Xperience is to demonstrate that state-of-the-art enactive systems can be significantly extended by using structural bootstrapping to generate new knowledge. This process is founded on explorative knowledge acquisition, and subsequently validated through experience-based generalization. In Xperience we are going to implement, adapt, and extend a complete robot system for automating introspective, predictive, and interactive understanding of actions and dynamic situations.

IntellAct (http://intellact.eu/)

In this project we address the problem of understanding and exploiting the meaning of manipulations in terms of objects, actions and their consequences for reproducing human actions with machines. This is in particular required for the interaction between humans and robots, in which the robot has to understand the human action and then transfer it to its own embodiment. IntellAct aims to provide the means to allow for this transfer, not by



Figure 4: An imitation learning system that can take into account forces and torques arising in tasks that involve contact with the environment.

copying the movements of the human but by transferring the human action on different levels, including action semantics. We will demonstrate the ability to understand scene and action semantics and to execute actions with a robot in two domains: in a laboratory environment (exemplified by a lab on International Space Station) and in an assembly process in an industrial context.

ACAT (http://www.acat-project.eu)

This project focuses on the problem how artificial systems (robots) can understand and utilize the information made for humans. For this, ACAT generates a dynamic process memory by the extraction and storage of action categories from large bodies of human compatible sources (text, images). Action categories are designed to include

the actual action-encoding, but also large amounts of context information ("background"). The ACAT system then uses action-categories to compile robot-executable plans. Execution benefits strongly from the rich context information present in the action-categories, which allows for generalization (for example, the replacement of objects in an action). It also permits us to specifically address the ambiguity, incompleteness and uncertainty in planning. Plans are grounded by perception and execution, which takes place with a robot. This leads to a life-long update process of the knowledge base.

In IntellAct we developed a new concept for the imitation learning which enables the consideration of forces and torques arising during the execution of the task. The developed technology is currently being transferred to industrial environments with an industrial partner.

The most important result of IntellAct in 2013 was the development of a new methodology for learning and the adaption of manipulation skills that involve physical contact with the environment. Pure position control is

unsuitable for such tasks because even small errors in the desired trajectory can cause significant deviations from the desired forces and torques. The proposed algorithm takes a reference Cartesian trajectory and the force/torque profile as the input and adapts the movement so that the resulting forces and torques match the reference profiles. Experimentally, we showed that the robot's performance can be significantly improved within a few iteration steps, compensating for vision and other errors that might arise during the execution of the task.

Among the important results of Xperience in 2013 was the development of a system that extends the framework of dynamic movement primitives with force/torque feedback, thereby bridging the gap from kinematic behaviours typically encoded by DMPs to dynamic behaviours. We proposed and evaluated a modulation approach that allows the interaction with objects and the environment. Through the proposed coupling of originally independent robotic trajectories, the approach also enables the execution of bimanual and tightly coupled cooperative tasks. We also proposed an approach for altering existing robot behaviours online, where a human coach interactively changes robot motion to achieve the desired outcome. Using hand gestures, the human coach can specify the desired modifications to the previously acquired behaviour. Another important line of research was how to improve visual object learning and recognition by exploiting the advantages of foveated vision. We showed that we can improve the performance of learning by using the manipulation capabilities of the robot and various resolutions of a foveated vision system.

In ACAT we are especially interested in Cartesian space representations of motor skills, as textual information usually refers to Cartesian space. We have therefore shown how dynamic movement primitives can be defined for non-minimal, singularity free representations of orientation, such as rotation matrices and quaternions. All of the advantages of DMPs, including ease of learning, the ability to include coupling terms, and scale and temporal invariance, can be adopted in our formulation. We have also proposed a new phase-stopping mechanism to ensure full movement reproduction in the case of perturbations.

Research in the area of humanoid and cognitive robotics is further conducted within a number of smaller projects supported by the Slovenian Research Agency and other international entities as well as with funding acquired in the frame of the young researchers program. In the frame of a bilateral project with ATR Computational Neuroscience Laboratories, Kyoto, Japan, funded by the Slovenian Research Agency and the Japan Society for the Promotion of Science, we performed a number of experiments in the area of humanoid robotics. All our projects focus on a better understanding of sensorimotor learning, visual processing, and lifelong learning in robotic systems, thus contributing to the overall vision of the group. We have published our results in prime robotics journals and at the most important robotics conferences, like Humanoids, IROS and ICRA, where we also organized two workshops in 2013.

III. Biocybernetics (Environmental Physiology and Ergonomics)

The biocybernetics group focuses primarily on research projects concerning the influence of extreme environmental factors on humans as well as the development and evaluation of technology and strategies to maintain safety and unhindered performance in such extreme environments.

Planetary Habitat Simulation (PlanHab)

The aim of this research program is to investigate the effect of a simulated planetary habitat environment on different human physiological systems. For technical reasons, the environment within future Lunar and Mars habitats will be hypobaric and hypoxic. Prolonged exposure to low gravity results in a deconditioning of vital physi-

A research program funded by the European Space Agency (ESA) Programme for European Cooperating States (PECS) and EU Framework program (FP7), which addresses the effects of longer exposure to combined inactivity/ unloading and hypoxia have been successfully completed at the Olympic Sport Centre Planica. Prolonged exposure to low gravity results in a deconditioning of vital physiological systems, and may consequently constitute a threat to the health of the astronauts. However, it is not known how prolonged exposure to both reduced gravity and hypoxia will affect health. For the purpose of this research programme we established a Planetary Habitat Simulation Facility at the Olympic Sport Centre Planica. The challenge of the project is in the complexity of the experimental interventions, whereby healthy humans are confined to a hypoxic environment during prolonged bedrest. Subjects have recently participated in three trials: hypoxic bedrest (simulated altitude 4000m), normoxic bedrest, and hypoxic ambulation. The effects of these

interventions were investigated in experiments concerning metabolic, cardiorespiratory, musculoskeletal, haematological, immunological and thermoregulatory functions. We anticipate that the new knowledge gained from these studies will also have clinical implications, since chronic hypoxia and bedrest constitutes a model of the underlying chronic condition experienced by patients suffering from respiratory insufficiency, cardiac diseases and obesity.

Central Sleep Apnea and Body Temperature Regulation in Normobaric versus Hypobaric Hypoxic Environments

Thus, aim of this study is to examine the acute and chronic effects of living at altitude on central sleep apnea, whether exposure to hypoxia will prevent the effective dilation of peripheral blood vessels in the evening, and whether these responses will delay the onset of sleep, ultimately affecting sleep quality and the likelihood of suffering mountain sickness or other adverse health outcomes. The results of this study will provide information for the assessment of clinical sleep function, particularly for populations with peripheral vascular disorders. The study

is supported by the European Space Agency, and is being conducted at the Concordia Antarctic Research station situated at an altitude equivalent to approximately 4000 m at the equator. The results of the study will be compared to the results obtained in studies conducted at a similar simulated altitude at the Olympic Sport Centre Planica, but in normobaric hypoxic conditions. In this manner we will contribute to the evaluation of the Equivalent Air Altitude Theory.

Hypoxia and Metabolic health

The weight loss observed during prolonged sojourns at high altitude does not appear to be entirely due to an imbalance between energy intake and expenditure. The observation that high-altitude exposure may lead to considerable weight loss has led to the suggestion that it might be beneficial to incorporate hypoxic training in weight-management programs for obese individuals. Studies have demonstrated that mild physical exercise in normobaric hypoxia causes a significantly greater weight loss in obese people than exercise in placebo hypoxic environment. To our knowledge, no systematic studies have been carried out to date regarding the treatment



Figure 5: Humanoid head used in experiments on object learning by manipulation and foveated vision.

of obesity and metabolic syndrom under hypoxic conditions. During prolonged sojourns to high altitude, factors which may contribute to weight loss include: dehydration, primary anorexia, lack of palatable food, detraining, and possibly direct effects of hypoxia on metabolism. We completed a series of studies, co-financed by Dutch industrial partner b-Cat, investigating the effect of 10-d sojourns in normobaric hypoxia, equivalent to a simulated altitude of 3200 m, on metabolism in combination with exercise training or without any activity. Specifically, the responses of plasma glucose, insulin, gut peptides, resting energy expenditure and satiety scores following a standard meal. Preliminary results indicate that one of the main contributors implicated in the observed weight loss is the elevated resting energy expenditure, and reduced appetite. Our current focus on this topic is the dose response to different levels of physical activity in hypoxia, coupled with an investigation of the effects of different hypoxic modalities on oxidative stress and cardiovascular health. In this regard we have established a collaboration with the Universities of Lausanne and Lyon.

Sleep architecture during hypoxic exposures

With colleagues from the Institute of Neurophysiology at University Clinical Centre Ljubljana we are investigating the effect of sleep architecture during prolonged exposure to hypoxia combined with different levels of activity. Research in this area is performed both under normobaric hypoxic conditions (Planica facility) and under hypobaric hypoxic conditions (Antarctic ESA research station). Our findings to date indicate that the main effect of hypoxia on sleep arise from changes in the frequency and magnitude of central sleep apnea.

Sleep temperature regulation

In addition to the polysomnographic recordings, we have also tested the theory that sleep onset is functionally linked with thermo-afferent feedback from cutaneous warm receptors. Our preliminary results confirm this theory, but have revealed that the hypoxia-induced vasoconstriction observed during the day disappears during the night. Thus our main studies in this area now focus on gaining a better understanding of this phenomenon through repeated measures and longitudinal designs.

Altitude retinopathy

Using a non-mydriatic fundus camera we have documented the diameter of retinal arterioles and venules at different stages of hypoxic exposure. Together with colleagues from the Eye Clinic at the University Clinical Centre, and the VITO Institute in Belgium we are currently analysing these scans to assess any hypoxia-induced vascular changes in the retina, which may be related to the onset of altitude retinopathy.

Field studies

In addition to our laboratory investigations, we continue to collaborate with high altitude Slovenian expeditions as well as with a number of national sport teams, assisting with their preparations and monitoring the effects of the high altitude exposures or altitude training regimens on various physiological systems and performance.

Development of diagnostic tool for determining susceptibility to freezing cold injury

In Slovenia, the main risk group for cold injury are alpinists participating in high-altitude expeditions. In collaboration with researchers from the Royal Institute of Technology (Stockholm, Sweden), we are running a research program, with two specific aims: i) to develop a diagnostic method to determine the susceptibility of individuals to cold injury; ii) to develop a training program to improve an individual's vascular response to a cold stimulus, thus



Figure 6: We are coordinating the research programme HASTE (Hypoxia: Altitude, Sleep & Temperature in Extreme Environments: Central sleep apnea and body temperature regulation in normobaric versus hypobaric hypoxic environments), supported by the European Space Agency (ESA), at the Antarctic research station Concordia

minimizing one's risk to cold injury. A series of laboratory and field studies have been conducted, examining the digit vascular response to cold-water immersion (cold-induced vasodilatation, CIVD), and the pattern of digit reperfusion following cold exposure using infrared thermography. We are currently evaluating the effect of several training programs, in terms of their effect on the CIVD response.

Evaluation of protective clothing (Desert Ensembles)

Soldiers on peacekeeping missions in desert regions must be able to sustain prolonged exposures to hot (45°C) and dry (10% relative humidity) environments, all while dressed in full combat gear. Our research program initially focused on the physiological responses of soldiers carrying loads in such environments. We have continued our work in this area, and have evaluated the efficacy of different technologies (i.e., ventilated vests) and/or strategies (i.e., work/rest schedules) in minimizing heat strain and improving performance in such environments. Together with colleagues from the Royal Institute of Technology we have continued this work to assess the impact of the next-to-skin layer on the thermal balance of soldiers in such environments. In addition, we have also investigated the effect of moisture content of the next-to-skin layer on predicted burn injuries during a simulated flash fire. With an industrial partner Lenzing (Austria) we have demonstrated that

increased moisture content of the next-to-skin layer provides added protection against burn injury. We are continuing our analysis to determine under what conditions the microenvironment moisture may lead to a scalding injury.

Thermal and nonthermal factors affecting exercise tolerance in the heat

Based on the Marie Curie IRSES grant on the "International cooperation for the advancement of research on the underlying systems of human thermoregulation" we initiated a research collaboration with the University of Cape Town. The project aims at advancing the current understanding of physiological responses to thermal stress and the main underlying mechanisms. The exchange of researchers between the two institutions allows for a significant transfer of knowledge, experimental techniques and ideas between the laboratories.

Some outstanding publications in the past three years

- Petrič, T., Gams, A., Babič, J., Žlajpah, L: Reflexive stability control framework for humanoid robots. Autonomous robots, 2013, vol. 34, no. 4, 347–361
- Peternel, L., Babič, J.: Learning of compliant human robot interaction using full-body haptic interface. Advanced robotics, vol. 27, no. 3, 2013
- Gams, A., Petrič, T., Debevec, T., Babič, J.: Effects of robotic knee exoskeleton on human energy expenditure. IEEE transactions on bio-medical engineering, ISSN 0018-9294, 2013, vol. 60, no. 6, 1636–1644
- 4. Schiebener, D., Morimoto, J., Asfour, T., Ude, A.: Integrating visual perception and manipulation for autonomous learning of object representations, Adaptive Behavior, vol. 21, no. 5, 328–345 (2013)
- Forte, D., Gams, A., Morimoto, J., Ude, A.: On-line motion synthesis and adaptation using a trajectory database, Robotics and Autonomous Systems, vol. 60, no. 10, 1327–1339 (2012)
- Debevec, T., Pialoux, V., Mekjavic, I. B., Eiken, O., Mury, P., Millet, G. P.: Moderate exercise blunts oxidative stress induced by normobaric hypoxic confinement. *Medicine and science in sports and exercise*, ISSN 0195-9131, 2014, vol. 46, no. 1, 33-41

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Awards and appointments

Marjeta Kramar Fijavž: Best University Teacher Award at Department of Civil Engineering, University 1 of Ljubljana, Faculty of Civil and Geodetic Engineering, awarded by the Student Council of the Faculty, Ljubljana, December 2013

Organization of conferences, congresses and meetings

- The 22nd International Workshop on Robotics in Alpe-Adria-Danube Region RAAD 2013, Portorož, Slovenia, 1. 11.-13.9.2013
- IntellAct Meeting, Ljubljana, Slovenia, 9. 9. 2013 2.

Patent granted

Igor Kovač, Borut Lenart, Bojan Nemec, Marko Scortegagna, Leon Žlajpah, Humanoid torso mechanism, 1. SI24099 (A), Urad RS za intelektualno lastnino, 31.12.2013.

INTERNATIONAL PROJECTS

- 1. Stimulators and Parts Foreign Buyers
- Asst. Prof. Aleš Ude
- 7FP IntellAct; Inteligent Observation and Execution of Actions and Manipulation European Commission Asst. Prof. Aleš Ude
- 7FP Xperience; Robots Bootstrapped through Learning from Experience European Commission
- Asst. Prof. Aleš Ude 7FP - ACAT; Learning and Execution of Action Categories European Commission
- Asst. Prof. Aleš Ude 7FP - CoDyCo; Whole-body Compliant Dynamical Contacts in Cognitive Humanoids European Commission Asst. Prof. Jan Babič
- 6. 7FP - ICARUS; International Cooperation for the Advancement of Researcher on the Undrelaying System of Human Thermoregulation European Commission
- Prof. Igor Mekjavić 7. 7FP - PlanHab: Planetary Habitat Simulation European Commission
- Prof. Igor Mekiavić
- Accelerated Development of Autonomous Behaviors for Humanoid Robots Slovenian Research Agency Asst. Prof. Aleš Ude

RESEARCH PROGRAM

Avtomation, Robotics and Biocybernetics 1 Prof. Igor Mekjavić

VISITORS FROM ABROAD

- Dr. Simon Hangl, University of Innsbruck, Austria, 7.-11. 1. 2013 1.
- Paul Canatella, Biran McAdams, W. L. Gore & Associates, Inc., Elkton, Maryland, USA, 2. 12.-14.1.2013
- Nora Beck Tan, W. L. Gore & Associates, Inc., Elkton, Maryland, USA, 13.-14. 1. 2013 3 Sabrina Langenmaier, W. L. Gore & Associates, Feldkirchen, Germany, 13.-14. 1. 2013 4
- 5.
- Dr. Tarsi Bali, Univesity of Athens, Greece, 17. 2.–6. 4. 2013 Anders Glent Buckt, BSc, SDU Odense, Denmark, 20.–22. 3. 2013 6.
- Dr. Nathalie Pattyn, Helio Fernandez, University of Brussels, Belgium, 17.-20. 4. 2013
- Ksavier Neyt, University of Brussels, Belgium, 17. 4.-4. 5. 2013 8
- Dr. Stylianos Kounalakis, University of Athens, Greece, 3. 5.-10. 5. 2013
- 10. Dr. Marietta Konstantonpoulo, Clinical Centre in Patras, Greece, 3.-10. 5. 2013
- 11. Prof. Sang- Ho Hyon, University of Ritsumeikan, Kyoto, Japan, 11.-14. 5. 2013

- **R&D GRANTS AND CONTRACTS**
- Dual Nature of Stem Cells in Cancer and Their Application in Therapy Prof. Igor Mekjavić
- 2 Learning, Analysis, and Detection of Motion in the Framework of a Hierarchical Compositional Visual Architecture Asst. Prof. Aleš Ude
- The Role of Small GTPases in the Regulation of Endosomal/Lysosomal Transport in Astrocytes
- Prof. Igor Mekjavić
- The Detection of Irregularities and Fraud in the Financing of the Public Health Services Dr. Marjeta Kramar Fijavž
- Development of a New Generation of Thermal Manikin for Evaluation of Personal Protective Equipment and Safety of Health in Extreme Working and Living Environmental Conditions (X-Termoman) Prof. Igor Mekjavić
- 6. Influence of Ski Width on Alpine Skiing Safety Asst. Prof. Bojan Nemec
- Zero and Reduced Gravity Simulation: The Effect on the Cardiovascular and Musculoskeletal Systems Prof. Igor Mekjavić
- Hypoxic Inactivity: Implications for Heart Failure, Respiratory Insufficiency and Obesity 8. Prof. Igor Mekiavić
- 9 On-line Learning and Adaption of Robot Skills to the Demonstrated Force Profiles Asst. Prof. Aleš Ude

NEW CONTRACT

- 1 Monitoring Foot Growth in Children UCS - Universal Customization System, d. o. o. Prof. Igor Mekjavić
- 12. Shingo Ando, Masaru Adachi and Yukio Nose, Yashawa, Japan, 13.- 15. 5. 2013
- 13. Dr. Jun Morimoto, Dr. Sang-Ho Hyon, Dr. Norikazu Sugimoto, 11.-15. 5. 2013
- Dr. Tomoyuki Noda, ATR Computational Neuroscience Laboratories, Kyoto, Japan, 14. 11.-15. 5. 2013
- 15. Dr. Emre Ugur, University of Innsbruck, Austria, 13.-15. 6. 2013
- 16. Dr. Elske Schabort, University of Cape Town, South Africa, 21. 7.-5. 8. 2013
- Dr. I-Ming Chen, Nanyang Technological University, Singapore, 13.–14. 9. 2013
 Dr. Norbert Krüger, SDU Odense, Denmark, 12.–13. 9. 2013
- 19. Dr. Emre Ugur, University of Innsbruck, Austria, 13.-14. 9. 2013
- 20. Dr. Andreas Holzbach, TU Munich, Germany, 16.-27. 9. 2013
- 21. Prof. Aleš Leonardis, University of Birmingham, United Kingdom, 30. 9. 2013
- 22. Prof. Hiroshi Ishiguro, ATR Kyoto, Japan, 11. 10. 2013



- 23. Prof. Henrik Sharfe, University of Aalborgu, Denmark, 11. 10. 2013
- 24. Shingo Ando, Yaskawa, Japan, 25. 10. 2013
- 25. Dr. Michael Mistry, University of Birmingham, United Kingdom, 14.-17. 11. 2013
- 26. Dr. Fares Abu-Dakka, University of Madrid, Spain, 4.-14. 12. 2013
- 27. Prof. Vincenzo Parenti-Castelli with students, University of Bologna, Italy, 23. 12. 2013

STAFF

Researchers

- 1. Asst. Prof. Jan Babič
- 2. Dr. Andrej Gams
- 3. Asst. Prof. Igor Kovač
- 4. Prof. Igor Mekjavić
- 5. Asst. Prof. Bojan Nemec
- 6. Dr. Anton Ružić
- 7. Asst. Prof. Aleš Ude

8. Asst. Prof. Leon Žlajpah, Head Postdoctoral associates

- 9. Dr. Fares Jawad Mohd Abu-Dakka, left 24.10.13
- 10. Dr. Tarsi Bali
- 11. Asst. Prof. Gregor Cigler*
- 12. Dr. Tadej Debevec
- 13. Dr. Denis Forte
- 14. Prof. Igor Klep
- 15. Asst. Prof. Marjeta Kramar Fijavž*
- 16. Dr. Shawnda Morrison, left 01.12.13
- 17. Dr. Tadej Petrič
- 18. Dr. Janez Šter, left 01.10.13
- Postgraduates
- 19. Robert Bevec, B. Sc.

BIBLIOGRAPHY

Roman Hribar, B. Sc.
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20. Miha Deniša, B. Sc.

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26. Rok Vuga, B. Sc.

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21. Aljaž Kramberger, B. Sc.

23. Adam Mc Donnell, B. Sc.

25. Barry Martin Ridge, B. Sc.

24. Luka Peternel, B. Sc.

Note: * part-time JSI member

Original Article

- 1. Fares Abu Dakka, Francisco Rubio, Francisco Valero, Vicente Mata, "Evolutionary indirect approach to solving trajectory planning problem for industrial robots operating in workspaces with obstacles", *Eur. j. mech. A, Solids*, vol. 42, pp. 210-218, 2013.
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- Giancarlo Bilancio, Cinzia Lombardi, Rado Pišot, Igor B. Mekjavić, Natale Gaspare De Santo, Maria Grazia Luciano, "Effects of prolonged immobilization on sequential changes in mineral and bone disease parameters: to the editor", *Am J Kidney Dis*, vol. 61, no. 5, pp. 845-847, 2013.
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- 3. Robert Bevec, Aleš Ude, "Object learning through interactive manipulation and foveated vision", In: *HUMANOIDS 2013*, IEEE-RAS International Conference on Humanoid Robots, October 15 -17, 2013, Atlanta, Georgia, USA, Danvers, IEEE, 2013, pp. 234-239.
- 4. Helena Chowdhury Haque, Jelena Velebit Marković, Nataša Radić, Vito Frančič, Igor B. Mekjavić, Ola Eiken, Robert Zorec, "A new approach to study properties of isolated preadipocytes following in vivo exposure to hypoxia", In: *Proceedings of Life in space for life on earth, 18-22 June 2012, Aberdeen*, (ESA SP (CD-ROM)), L. Ouwehand, ed., Noordwijk, ESA Communications, 2013.
- Miha Deniša, Tadej Petrič, Tamim Asfour, Aleš Ude, "Synthesizing compliant reaching movements by searching a databaseof example trajectories", In: *HUMANOIDS 2013*, IEEE-RAS International Conference on Humanoid Robots, October 15 -17, 2013, Atlanta, Georgia, USA, Danvers, IEEE, 2013, pp. 540-546.
- 6. Miha Deniša, Aleš Ude, "New motor primitives through graph search, interpolation and generalization", V: Frontiers of intelligent autonomous systems: [selected papers from the 12th International Conference on Intelligent Autonomous Systems (IAS-12), Jeju, Korea, June 26-29, 2012], (Studies in computational intelligence, 466), Sukhan Lee, ur., Kwang Y. Lee, ur., Jangmyung Lee, ur., Heidelberg, New York, Springer, cop. 2013, str. 137-148.
- 7. Andrej Gams, Jesse van den Kiebooma, Florin Dzeladini, Auke Jan Ijspeert, "Stable real-time full body motion imitation on the COMAN humanoid robot", In: *Proceedings*, 22nd International Workshop on Robotics in Alpe-Adria-Danube Region [also] RAAD 2013, September 11-13, Portorož, Slovenia, Bojan Nemec, ed., Leon Žlajpah, ed., 1st ed., Ljubljana, Jožef Stefan Institute, 2013, pp. 25-32.
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INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

 Đani Juričić, Matej Gašperin, Bojan Musizza, Gregor Dolanc, Igor B. Mekjavić, "A system for model-based quality assessment of burnprotective g arments", In: *Case studies in control: putting theory to work*, (Advances in industrial control), Stanko Strmčnik, ed., Đani Juričić, ed., London [etc.], Springer, 2013, pp. 257-285.

PATENT APPLICATION

1. Igor Kovač, Borut Lenart, Bojan Nemec, Marko Scortegagna, Leon Žlajpah, *Humanoid torso mechanism*, EP2676776 (A1), European Patent Office, 25.12.2013.

PATENT

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MENTORING

- 1. Denis Forte, Generalization of libraries of robot movements using statistical methods: doctoral dissertation, Ljubljana, 2013 (mentor Aleš Ude).
- 2. Miroljub Jakovljević, Effect of inert gases on thermal stimuli sensation: doctoral dissertation, Ljubljana, 2013 (mentor Igor B. Mekjavić). 3. Tadej Petrič, Advanced robot control using adaptive oscillators:
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DEPARTMENT OF SYSTEMS AND CONTROL

E-2

The department is engaged in the analysis, control and optimization of systems and processes. The activities of the department are focused on the research of new methods and algorithms for automatic control, the development of procedures and tools to support the design and construction of control systems, the development of specific measurement and control modules, and the development and construction of complete systems for the control and supervision of machines, devices and industrial processes.

Basic and applied research

The basic and applied research in 2013 was devoted to three sub-areas: methodologies for analysis and control systems design; tools and building blocks for implementation; and applied research in the priority problem domains. The sub-area methodologies for analysis and control systems design included three topics.

The first topic addressed modeling and identification of nonlinear and complex dynamical systems. The research in the dynamic systems modelling of Gaussian process models was directed towards the on-line training Head: and application of the on-line training for on-line control. The identification of Gaussian process models was used Dr. Vladimir Jovan for the modelling of biological and environmental systems (Figure 1). A key feature of modern condition monitoring systems is the ability to predict the remaining useful life of the system or its components. To achieve this, we focus on the development of system identification algorithms for model-based prognostics and health management (PHM). We have developed a prognostics algorithm, which merges a sequential Monte-Carlo approach with a classical Kalman filter. The algorithm was applied to predict failures in both mechanical and electro-chemical systems.

The second topic was *advanced control*. We have continued the development and robustification of methods for the implementation of the simplified parametric predictive controller in practical control applications. We have implemented an improvement of a cascade scheme of magnetic plasma control for the Iter fusion tokomak reactor, where an additional feedback loop in charge of returning the vertical plasma position to the origin was introduced between the inner loop of vertical stabilisation and the outer loop of plasma current and shape control.

The third topic of interest was condition monitoring and fault diagnosis. Research in the area of condition monitoring has resulted in novel approaches to the robust diagnosis and prognosis of rotational machines and drives under incomplete information about variable operating conditions. The problem is notoriously difficult and relevant for practice. New results rely on the stochastic modelling of structural excitations that emerge from complex interactions between rotating and stationary parts by means of point processes. In addition, a new algorithm for detecting distributed faults in bearings from vibrational recordings has been developed. The solution to this nontrivial problem is applicable to the faults due to, e.g., electro-erosion in bearings. The most notable contribution in the area is related to the completed experimental prototype of a diagnostic and prognostic platform for rotational machines and successful implementation on three different industrial sites in Slovenia and abroad (Figure 2). The platform relies on an innovative holistic concept of the distributed sensor network, which allows for partial local signal processing, data fusion from different sensors, selftuning of decision thresholds, remote configuration as well as integration Figure 1: The predicted mean value and 95% confidence interval of with other information systems in the enterprise.

In the area tools and building blocks for implementation the MAGICS

methodology for the development and automatic generation of process control software has been further developed. An experimental industrial prototype of an environment for this methodology has been developed, which supports the industrial practice of modelling and, partly, the automatic generation of the procedural part of the software for demanding process control systems.

In the field of production control, we were developing a software tool named ProOpter that enables the analysis of production dynamics using advanced methods like data mining, data reduction, determination of relevant manipu-





ozone concentration for 9 August 2008 from GP model



Figure 2: Scheme of the prototype of diagnostics & prognostics platform

lated variables and production performance indicators model identification (Figure 3). The obtained models enable the prediction and optimization of the production dynamics.

A reliable estimate of the remaining useful life is getting to be one of the most significant requirements in modern maintenance. We continued our research of a class of data-driven methods that rely on stochastic models derived from run-to-failure experiments performed on an appropriate set of similar items of equipment. A method employing entropy indices calculated from vibrational records has been further improved. Dynamic relations between indices and time-to-failure are described by Gaussian Process Models with truncated Gaussian distributions, which results in efficient new algorithms.

In 2013 we continued working on the diagnostics of PEM fuel cells with the use of impedance measurements. The main focus was on a procedure for collecting the impedance information. In this manner we developed a procedure for the estimation of the instantaneous PEM fuel-cell impedance, which is based on PRBS perturbation signals and the continuous wavelet transform. The procedure provides the means for an approximately five-times faster estimation of the impedance compared to conventional approaches.

In the area of fuel-cell models development the main objective was to build a Matlab/Simulink model of the HyPM ® HD 8-200 Fuel-cell-based

power unit, purposed for testing control approaches and the optimization of power management. In the model, a combination of the use of the measured static characteristics and tuning of the physical equations that describe processes in the FC stack, as well as the Balance of Plant (BoP) components (blower, pumps, etc.) in the system. During this year the model has been extended with the stack temperature influence to internal resistance and output voltage. In parallel a load study and the assessment of battery choice for a FC-based APU has been made.

Applied research in the priority problem domains was the third sub-area of our interest. In this frame a substantial part of our activities was devoted to the development of the specific control systems described below.

In the frame of the Slovenian Research Agency's project on energy optimisation, new dynamic models of chillers for the purpose of energy consumption optimisation have been developed.

Control of wastewater treatment plants is our traditional research area. In cooperation with the company Kolektor Sinabit d.o.o., in 2013 we have developed a feed rate control of the anaerobic reactor for organic waste removal and biogas production. The proposed control adjusts the feed rate of the substrate based on measurements of the volatile fatty acids and acetate in the reactor. The control enables stable biogas production and prevents acidification of the process. Control was tested on the anaerobic reactor pilot plant.

In the frame of the Eurostars project ProDISMon we started with the development of algorithms aimed to improve the reliability of distributed condition monitoring systems by means of an on-line assessment of the quality



Figure 3: Placement scheme of a software tool ProOpter

of the acquired data as well as the fusion of data from various sensory inputs. In recent years, a part of our work was focused on the area of *fuel cells*. In 2011 we started cooperation on the 7th European project FCGEN-Fuel Cell Based On-board Power Generation. The objective of the FCGEN project is the development and demonstration of an auxiliary power unit (APU) for trucks, which uses an auto-thermal reformer to produce hydrogen from fuel and a fuel-cell stack for the electric energy production. In 2013 most of the process reactors for diesel conversion and reformate clean-up have been built and tested. Our group had two main work tasks. First, was the development of the complete APU control system and second was the development of the APU power-conditioning components. For the control system first the PLC version and HMI were finalized, and partially tested during the reactor tests. During the second half of the year the focus was on the development of the main controller, APU ECU, and the transfer of the control code from the PLC to the embedded controller. Within the power-conditioning task the prototype of the DC/DC converter and the power supply for the BoP component has been developed, built and tested.

Within the second 7th European project *FluMaBack-Fluid Management* component improvement for Back up fuel cell systems the control line for the final quality control of blowers for fuel-cell systems has been designed. It consists of two modules. The first module examines the bearing quality by analysing the sound emissions. The second module examines the vibrational and electrical signals. The overall quality is estimated based on the calculated features.

R&D projects for industry and other users

A substantial part of the department's R&D activities for industry and other users is conducted within the project Competence Centre for Advanced Control Technologies, which has been concluded in 2013. Within the programme of the Competence Centre for Advanced Control Technologies our department members developed a number of

innovative technological solutions in cooperation with industrial partners. The developed control tools and building blocks include advanced control algorithms that were implemented within the software tools of the Inea and Kolektor Sinabit companies for the easy implementation of advanced control in industrial processes. In addition, an industrial prototype of a tool for the model-driven development of the process control software was developed. In the field of a smart factory, a ProOpter production dynamics analyser and optimiser was developed and tested in batch production at our partner Helios, while the platform for on-line condition monitoring of industrial assets, implemented at the company Litostroj Power, was integrated with the existing information system in the company. The control solutions for the efficient use of energy include the design of an algorithm for the optimal selection of heating and cooling systems in smart buildings that was implemented and tested by the company Goap, while the improved control of the anaerobic fermenter in the production of biogas was implemented Figure 4: "Heavy-duty" value drive for Danfoss Trata d.o.o. by Kolektor Sinabit and tested on a pilot-scale batch reactor. A particular

challenge in the field of energy production is the control of a fusion reactor. Within the realistic demonstrator of controlling plasma position, which was designed by the company Cosylab, an improved control solution based on a predictive controller was developed for plasma position control. Finally, within this programme our department members are planning to submit two patent applications and two innovations as leading partners.

Another important part of our activities is also devoted to direct cooperation with various companies.

In the project for Danfoss Trata d.o.o., the hardware and the firmware for "heavy-duty" motor drives have been developed (Figure 4). The drives are now in a trial production phase at Danfoss Trata, d.o.o. The drives have an anti-oscillation function that increases the expected lifespan of the drives and decreases the energy consumption. In addition to the heavy-duty drives, the concept of so-called "integration drives" has been developed and tested as well. Integration drives are used for tighter control of the output water temperature from heat exchangers.

An online estimation of the remaining useful life of electromotors is a challenging task. In the company Domel d.o.o. we developed and installed a line for the long-life testing of electronically commutated motors. The installed measuring equipment allows sufficiently accurate data acquisition and local data processing as well as an estimation of the remaining useful life. The final goal is the development of an embedded module for the estimation of the remaining useful life that will be an integral part of the final product.

In collaboration with the Centre of Excellence Low-carbon technologies, special DC/DC converters have been finalised and delivered to a number of national and European customers.

Publication of the book "Case Studies in Control - Putting Theory to Work"

The book entitled "Case Studies in Control - Putting Theory to Work" appeared in 2013 in the Springer series "Advances in Industrial Control". The book editors Prof. Dr. Stanko Strmčnik and Prof. Dr. Đani Juričić raised the topic of advanced control based on a number of case studies presented by our department members. The book summarizes the long-standing efforts and knowledge of our department in the field of the research of advanced control methods and their transfer to industrial practice. Case Studies in Control presents a framework to facilitate the use of advanced control concepts in real systems based on two decades of research and over 150 successful applications for industrial end-users from various backgrounds.

Educational and training activities

Some members of the department are giving lectures and practical courses at different faculties and universities: the Faculty of Electrical Engineering, University of Ljubljana, the Faculty of Logistics, University of Maribor, the University of Nova Gorica and the "Jožef Stefan" International Postgraduate School. They also act as supervisors of Ph.D. students.





Figure 5. Cover of the book Case Studies in Control -Putting Theory to Work

Some outstanding publications in the past year

- 1. Kocijan, J., Hvala, N.: Sequencing batch-reactor control using Gaussian-process models. *Bioresource technology*, ISSN 0960-8524, vol. 137, 340–348
- 2. Hvala, N., Kukanja, D.: Modelling and simulation of semi-batch polymerisation reactor for improved reactants dosing control. *Simulation modelling practice and theory*, ISSN 1569-190X, vol. 33, no. 1, 102–114
- Lukman, T., Godena, G., Gray, Jeffrey G., Heričko, M., Strmčnik, S.: Model-driven engineering of process control software beyond device-centric abstractions. *Control engineering practice*, ISSN 0967-0661, vol. 21, no. 8, 1078–1096
- 4. Petelin, D., Grancharova, A., Kocijan, J.: Evolving Gaussian process models for prediction of ozone concentration in the air. *Simulation modelling practice and theory*, ISSN 1569-190X, vol. 33, 68–80
- Glavan, M., Gradišar, D., Atanasijević-Kunc, M., Strmčnik, S., Mušič, G.: Input variable selection for model-based production control and optimisation. *The international journal of advanced manufacturing technology*, ISSN 0268-3768, 2013, vol. 68, no. 9/12, 2743–2759
- Glavan, M., Gradišar, D., Strmčnik, S., Mušič, G.: Production modelling for holistic production control. *Simula*tion modelling practice and theory, ISSN 1569-190X, jan. 2013, vol. 30, 1–20

The most important achievements in the past year

- 1. The book "Case Studies in Control Putting Theory to Work" edited by Prof. Dr. Stanko Strmčnik and Prof. Dr. Đani Juričić was published in the Springer series "Advances in Industrial Control".
- 2. The article on modelling and control of polymerization process has been ranked among the most downloaded articles in Computers & Chemical Engineering Journal.
- 3. The first dedicated DC/DC converters for fuel-cell systems have been sold on the European market.
- 4. Successful completion of a multi-annual project "Competence Centre for Advanced Control Technologies" where the department E2 was involved in several development subprojects.
- 5. Successful completion of a multi-annual work within the "Centre of Excellence Low-carbon technologies" where we were in charge for the research on the field of hydrogen technologies.

Awards and appointments

 Nadja Hvala: The article "Modelling, simulation and control of an industrial, semi-batch, emulsion-polymerization reactor" in Computers and Chemical Engineering Journal has according to Elsevier more than 500 downloads. It has been identified as one of the most downloaded articles in this journal in the period from Sept. 2012 - Aug. 2013 and has received a certificate for this contribution.

INTERNATIONAL PROJECTS

- Production of DC/DC Converters PowerCell Sweden AB Dr. Janko Petrovčič
- 2. 7FP FCGEN; Fuel Cell Based On-board Power Generation European Commission
- Dr. Boštjan Pregelj 3. 7PP - FLUMABACK; Fluid Management Component Improvement for Back up Fuel Cell
 - Systems European Commission
 - Dr. Pavle Boškoski
- CERACON; Integration and Control of Liquid Fuel processor based on Ceramic Micro-Systems ESA/ESTEC.
 - Dr. Gregor Dolanc
- COST IC0806, IntelliCIS; Intelligent Monitoring, Control, and Security of Critical Infrastructure Systems COST Office Dr. Nadja Hvala

RESEARCH PROGRAM

1. Program Systems and Control Prof. Đani Juričić

R&D GRANTS AND CONTRACTS

- Prognostics and health management of mechanical drives based on novel MEMS sensor networks Prof. Đani Iuričić
- Development and implementation of a method for on-line modelling and forecasting of air pollution
- Prof. Juš Kocijan
 Optimisation of energy cost for refrigeration systems in shopping malls Asst. Prof. Damir Vrančić
- 4. On-line System Identification for Model-Based Prognostics and Health Management Dr. Matej Gašperin
- Competence Centre for Advanced Control Technologies: CC ACT Asst. Prof. Damir Vrančić
- Probasensor: EUROSTARS; Probalistic Bayesian Soft Sensor A Tool for On-line Estimation of the Key Process Variable in Cold Rolling Mills Prof. Đani Juričić

NEW CONTRACTS

- 1. Process Control Software Development Methodology Inea, d. o. o.
- Giovanni Godena, M. Sc.
 Prognostics and Health Management of Mechanical Drives Based on Novel MEMS Sensor Networks
- Domel, d.o.o. Prof. Đani Juričić
Development and Implementation of a Method for On-line Modelling and Forecasting of Air Pollution MEIS environmental services, d.o.o. Prof. Juš Kocijan

VISITORS FROM ABROAD

1. Prof. Diego Galar, Luleå University of Technology, Luleå, Sweden, 2.-6. 9. 2013

STAFF

Researchers

- 1. Dr. Gregor Dolanc
- 2. Dr. Samo Gerkšič
- 3. Giovanni Godena, M. Sc.
- 4. Dr. Dejan Gradišar
- 5. Dr. Nadja Hvala
- 6. Dr. Vladimir Jovan, Head
- Prof. Đani Juričić
 Prof. Juš Kocijan
- Prof. Jus Kocijan
 Dr. Bojan Musizza
- 10. Dr. Janko Petrovčič
- 11. Prof. Stanislav Strmčnik
- 12. Asst. Prof. Damir Vrančić
- 13. Dr. Darko Vrečko
- Postdoctoral associates
- 14. Dr. Pavle Boškoski
- 15. Dr. Matej Gašperin

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 Optimisation of Energy Cost for Refrigeration Systems in Shopping Malls Entia, d.o.o. Asst. Prof. Damir Vrančić

- 2. Asst. prof. Václav Šmídl, University of West Bohemia, Plzen, Czech Republic, 2.-4. 10. 2013
- 16. Dr. Marko Nerat 17. Dr. Matija Perne 18. Dr. Boštjan Pregelj Postgraduates 19. Andrej Debenjak, B. Sc. 20. Boštian Dolenc, B. Sc. 21. Miha Glavan, B. Sc. 22. Dejan Petelin, B. Sc 23. Martin Stepančič, B. Sc. 24 Aleš Svetek M Sc Technical officers 25. Stanislav Černe, B. Sc. 26. Primož Fajdiga, B. Sc. Technical and administrative staff 27. Maja Janežič, B. Sc 28. Miroslav Štrubelj

ORIGINAL ARTICLE

- 1. Darko Aleksovski, Juš Kocijan, Sašo Džeroski, "Model tree ensembles for modeling dynamic systems", In: Discovery science: 16th International Conference, DS 2013, Singapore, October 6-9, 2013, proceedings, *Lect. Notes Comput. Sci.*, vol. 8140, pp. 17-32, 2013.
- 2. Darko Belavič, Marko Hrovat, Gregor Dolanc, Kostja Makarovič, Marina Santo-Zarnik, "Design and fabrication of an LTCC structure for a microceramic combustor: invited paper", *J. microelectron. electron. packag.*, vol. 9, no. 3, pp. 120-125, 2013.
- Andrej Debenjak, Matej Gašperin, Boštjan Pregelj, Maja Atanasijević-Kunc, Janko Petrovčič, Vladimir Jovan, "Detection of flooding and drying inside a PEM fuel cell stack", *Stroj. vestn.*, vol. 59, no. 1, pp. 56-64, Jan. 2013.
- Andrej Debenjak, Bojan Musizza, Matej Gašperin, Janko Petrovčič, "Diagnostični modul za gorivne celice s protonsko prevodno membrano", *Ventil (Ljubl.*), vol. 19, no. 3, pp. 200-206, jun. 2013.
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- Miha Glavan, Dejan Gradišar, Maja Atanasijević-Kunc, Stanko Strmčnik, Gašper Mušič, "Input variable selection for model-based production control and optimisation", *Int. j. adv. manuf. technol.*, vol. 68, no. 9/12, pp. 2743-2759, 2013.
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- 9. Ulf Jeppsson *et al.*, (17 avtorjev) "Benchmark simulation models, quo vadis?", *Water sci. technol.*, vol. 68, no.1, pp. 1-15, 2013.
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- Juš Kocijan, Nadja Hvala, "Sequencing batch-reactor control using Gaussian-process models", *Bioresour. technol.*, vol. 137, pp. 340-348, jun. 2013.

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REVIEW ARTICLE

1. Ingrid Petrič, Dejan Gradišar, Miha Glavan, Stanko Strmčnik, "Ključni kazalniki za merjenje uspešnosti proizvodnje", *Uporab. inform. (Ljubl.)*, vol. 21, no. 2, pp. 95-106, apr./maj/jun. 2013.

SHORT ARTICLE

 Matej Gašperin, Klemen Žagar, Drago Bokal, Klemen Strniša, Gašper Pajor, L. Medeiros-Romao, D. Vandeplassche, "Predictive diagnostics for high-availability accelerators", *Control sheet*, vol. 16, no. 9, pp. 2'3, 2013.

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 Juš Kocijan, "Incorporating knowledge about model structure in the identification of Gaussian-process models", In: Recent advances in telecommunications, signals and systems: proceedings of the 12th International Conference on Data Networks, Communications, Computer (DNCOCO '13), proceedings of the 12th International Conference on Non-Linear Analysis, Non-Linear Systems and Chaos (NOLASC '13), proceedings of the 9th International Conference on Dynamical Systems and Control (CONTROL '13), proceedings of the 6th International Conference on Sensors and Signals (SENSIG '13), proceedings of the International Conference on Visualization, Imaging and Simulations (VIS '13), Marc 21-23, 2013, Lemesos, Cyprus, (Recent advances in electrical engineering series, 10), Andreas Kanarachos, ed., [S. l.], WSEAS, 2013, pp. 124-129.

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- 1. Pavle Boškoski, Đani Juričić, "Detection of bearing faults based on inverse Gaussian mixtures model", In: *Surveillance 7: international conference: October 29-30, 2013, Chartres, France, Chartres, Institute of Technology, 2013, 12 pp.*
- 2. Pavle Boškoski, Đani Juričić, "MIMOSA OSA-EAI standard za E-Vzdrževanje", In: Zbornik osme konference AIG'13 Avtomatizacija v industriji in gospodarstvu, 4. in 5. april 2013, Maribor, Slovenija, Boris Tovornik, ed., Nenad Muškinja, ed., Milan Rotovnik, ed., Maribor, Društvo avtomatikov Slovenije, 2013, 7 pp.
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- 6. Andrej Debenjak, Matej Gašperin, Janko Petrovčič, "On-line tracking of fuel cell system impedance using extended Kalman filter", In: *Proceedings of the PHM2013, 2013 Prognostic and System Health Management, 8-11 September 2013, Milano, Italy,* (Chemical engineering transactions, vol. 33, 2013), Milano, AIDIC, 2013, vol. 33, pp. 1003-1008, 2013.
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- 12. Samo Gerkšič, Boštjan Pregelj, Stanko Strmčnik, Aleš Šink, Tadej Jerovšek, Aleksander Pregelj, Igor Steiner, "Aplikativna izvedba poenostavljenega eksplicitnega prediktivnega regulatorja na pilotni napravi", In: Zbornik osme konference AIG'13 Avtomatizacija v industriji in gospodarstvu, 4. in 5. april 2013, Maribor, Slovenija, Boris Tovornik, ed., Nenad Muškinja, ed., Milan Rotovnik, ed., Maribor, Društvo avtomatikov Slovenije, 2013, 7 pp.
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PATENT APPLICATION

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Mentoring

1. Gabrijel Peršin, *Fault detection and localization of mechanical drives based on data fusion techniques:* doctoral dissertation, Ljubljana, 2013 (mentor Jožef Vižintin; co-mentor Đani Juričić).

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. The main research areas are the following: data analysis with an emphasis on text, web and cross-modal data, scalable real-time data analysis, machine learning, analysis and modelling of large networks, visualization of complex data, semantic technologies, language technologies, reasoning methods and knowledge management. The Artificial Intelligence Laboratory has employees and students with an international background and with expertise in different areas of artificial intelligence. In addition to having their research results published in international publications, they have also developed several software tools for multimodal data analyses. Some of these tools are: Text-Garden, a suite of text mining tools; OntoGen (http://ontogen.ijs.si/), a tool for ontology learning; Document-Atlas (http://docatlas.ijs.si/), a tool for complex visualization; Atlas of Slovenian Science (http:// scienceatlas.ijs.si/), a web portal for analyzing the scientific community; Enrycher (http://enrycher. ijs.si/), a system for semantic enrichment of textual data; SearchPoint (http://searchpoint.ijs.si/), a portal for visual and contextualized Web browsing; OntoPlus, a methodology for semi-automatic Prof. Dunja Mladenić ontology extension; Contextify (http://contextify.net/), a tool for contextualized e-mail and contact management; NewsFeed (http://newsfeed.ijs.si/), a clean, continuous, real-time aggregated stream of semantically enriched news articles from RSS-enabled sites across the world; iDiversiNews (http:// aidemo.ijs.si/diversinews/) a system for processing and visualizing news; Event registry (http:// eventregistry.org/) a system for identifying mentioned world events in the news. The laboratory's strategy is to combine scientific excellence and strong industrial collaboration and to transfer research results into real-world business environments.

In the last 10 years, members of the Artificial Intelligence Laboratory successfully completed 32 EU projects, of which 5 were concluded in 2013. In addition, we were involved in another 12 EU FP7 projects in 2013, including 3 Networks of Excellence covering three complementary research areas: statistical data modelling and machine learning, language technologies and semantic technologies. Among our activities on national projects, we should

emphasize our involvement in three national application projects and the successful conclusion of two competence centers.

In the area of statistical data modelling and machine learning, we have contributed Big Data Tutorial at three international conferences: ISWC, WWW, ICDM (Marko Grobelnik, Blaž Fortuna, Dunja Mladenić), Topological Data Analysis Tutorial at the international conference ICML-2013 (Primož Škraba) and an invited course on Big Data Analytics at the Brazilian Machine Learning and Knowledge Discovery in Databases School (Marko Grobelnik). In the EU FP7 project XLike (Cross-lingual Knowledge Extraction) coordinated by our department, we have developed technology for the real-time cross-lingual linking of news articles across languages. This allows us to identify news stories in one language and observe when and how these stories spread across language barriers. Cross-lingual linking was successfully tested on the Bloomberg.com website, where it provided additional local context to readers (i.e., German or Italian) while reading Bloomberg news articles in English. In the EU FP7 project TOPOSYS (Topological Complex Systems) coordinated by our department, we have made significant progress in understanding the underlying mathematical foundations of multi-scale dynamic systems, in particular using topological tools. Some examples include understanding behaviors such as periodicity or more generally, recurrence in high-dimensional configuration spaces as well as more abstract space such as feature spaces; understanding the statistics of invariants/features as a method to formalize the notion of noise in an experimental setting and finally, transitioning from local to global information in a multiscale



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Figure 1: Science Atlas portal for visualization of Slovenian research community based on publications and projects (showing a collaboration graph for a selected researcher from computer science).

Primož Škraba had an invited talk "A Topological Model of Recurrence" at the Israeli Statistics Association Annual Meeting 2013.

manner. In the EU FP7 project *Symphony (Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy)* our work is mainly focused on developing tools and approaches for nowcasting. We have been working on establishing social media monitoring data infrastructure, tracking cross-lingual information and opinion diffusion, definition and development of social-media-based expectations indicators.

In the areas of **text and network analysis** and **language technologies**, we have organized "Knowledge Extraction from Text" Workshop at the international conference NIPS-2013. We have successfully concluded the EU FP7 Network of Excellence on Linguistics *METANet (Net Technologies for the Multilingual European Information*)



Figure 2: Science Atlas portal showing a collaboration graph in chemistry (based on research publications).

Society), providing a detailed expert analysis and assessment of the current situation of language resources and technologies for Slovenian (http:// www.meta-net.eu/whitepapers/volumes/slovene) and a Strategic Research Agenda for Multilingual Europe 2020 (http://www.meta-net.eu/sra). The results also include a network of repositories (http://www.meta-share.org/) of language data, tools and related web services documented with high-quality metadata, aggregated in central inventories, allowing for uniform search and access to resources now includes Slovenian language resources and applications. The European Social Fund project *Communication in Slovenian* was completed and resulted in a number of important Slovenian language resources, language technology applications and web portals. Text corpora include a 1.2-billion-word corpus of written texts Gigafida, a 100-million-word balanced corpus Kres, a 1-million-word spoken corpus Gos and a corpus of transcribed school essays Šolar (http://eng.slovenscina. eu). These databases can be explored online by using newly developed web

concordancers. Lexical data includes a lexical database with semantic, syntactic, collocation and other data, and the Slovenian lexicon Sloleks where inflectional paradigms for more than 100,000 Slovenian words can be found. Some basic language technology applications were developed that were needed for the computer processing of text in the Slovenian language, such as Slovenian tagger and parser. We have also concluded the EU FP7 project *LTWeb*, where we are participating in the standardization process of natural language processing service providers. We have successfully concluded the *Slovenian Science Atlas*, a national project, publically launching the available portal for searching and visualizing research collaboration and competences of Slovenian researchers. We have concluded the EU FP7 project *RENDER (Reflecting Knowledge Diversity)* where we have developed an iPad application iDiversiNews enabling the visualization of a live stream of news articles including an automatic summarization and opinion-mining application. In our new EU FP7 project *Sophocles (Self-Organised information PrOcessing, CriticaLity and Emergence in multilevel Systems)*, we have been working on processing social media data (Twitter, news) with the goal of validating the theoretical models developed in the project. The main phenomena of interest are the emergence of scales in the data as well as the detection of critical events that drastically change the dynamics of the system.

In the area of **semantic technologies**, we contributed the Internet of Things Tutorial at the international conference ISWC-2013 (Marko Grobelnik and Carolina Fortuna) and a keynote talk ESWC Summer School on Semantic technologies 2013 (Marko Grobelnik). We have continued work on methods for measuring concept similarity in ontologies, where the experimental evaluation was performed on DBPedia, OpenCyc ontology and on the WordNet lexical database. Within *Planet Data (Intelligent Information Management)*, a EU Network of Excellence, we have collected a large body sensor of data from publicly available services in London and Madrid that

Marko Grobelnik had an invited talk "Introduction to Big Data" at the European Data Forum 2013.

have been processed as streams using the MS StreamInsight and Esper tools with the purpose of detecting events as described in the 'Smart City' use case in PlanetData. In collaboration with the Institute's Communication Systems Department (E6), we have additionally investigated techniques for cleaning and repairing sensor data. The second line of work was concerned with text

streams, for which best practices and lessons learnt regarding the development of a real-time infrastructure have been developed. We also focused on using the News Storyline Ontology for annotating text streams for the 'New Registry' use case. In our new EU FP7 project *ProaSense (The Proactive Sensing Enterprise)* we are developing tools and approaches for forecasting future undesired events in the production process to enable a reaction to them beforehand. The project is one of the early adopters of a shift from reactive to proactive computing. Our new FP7 EU project *XLime (Cross-Lingua, cross-Media knowledge extraction)* is dedicated to fusing the knowledge from different dimensions of media content providing a near-real-time continuously updated and comprehensive view on knowledge diffusion across media. We are developing methods for the analysis of information derived

from various media channels, such as audio, video, text and social media as a first step towards the development of a real-time comprehensive view on knowledge diffusion across media and languages.

Knowledge management includes research and development by using methods and tools from a broader Artificial Intelligence area in real business settings. Following the invitation, we have organized a workshop for European anti-corruption agencies "EPAC/EACN Technical Seminar". The aim of the FP7 EU project NRG4Cast (Energy Forecasting) coordinated by our department, is the development of real-time management, analytics and forecasting services for energy distribution networks in urban/rural

Together with the Centre for Knowledge Transfer in Information Technologies, we received the World Summit Award (WSA) for Videolectures. net. Among 200 WSA winners from the last decade, 8 all-time bests were selected; VideoLectures.Net was selected as the winner in the "e- Science & Technology" category.

communities. Our work is focused on analyzing multimodal data streams from the energy domain. During the first year of the project, we have obtained and integrated sensor data streams and global services into an analytical platform, where analytical methods for data cleaning and fusion were applied. The first integrated prototype was released and validated by NRG4Cast case study partners: IREN, CSI and Envigence. In the FP7 EU project MobiS (Personalized Mobility Services for energy efficiency and security through advanced Artificial Intelligence techniques) we have developed services for traffic data collection, cleaning and fusion, used by the traffic-prediction services, which are also being developed. Part of this is a novel approach to the incremental decision-tree learning on data streams. We have also extended the Cyc ontology to be used within the traffic domain and exploited the Cyc reasoner to behave as an expert system, helping operators in the traffic call center (AMZS). We developed a

novel knowledge-capture service, which is being used to populate the traffic knowledge base extension mentioned before. All these services together serve as a traffic platform, which is currently used by the call-center expert system and custom mobile application prototype (Mobis Commuting Assistant) with the idea to help the daily commuters on their travels. In the FP EU project Mediamixer (Community set-up and networking for the remixing of online media fragments) we have been working on the use of fragmented media content.

Promotion of science is continually present in the efforts of the Artificial Intelligence Laboratory. We have been organizing a touring exhibition about female PhD holders from the area of computer science in Slovenia since 2006, thereby promoting the role of women in science (http://ScienceWithArt.ijs. si/). Our activities on TransLectures (Transcription and Translation of Video Lectures), a EU FP7 project, where we collaborate with the Centre for Knowledge Transfer in Information Technologies (CT3) on the automated subtitling and translating of video recordings, were focused on developing innovative tools for the automatic transcription and translation of educational video material. Together with 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 the main organizer and supporter of the annual national ACM Computer Science Competition for secondary-school students; this year, more than 200 students participated in the competition. Following the invitation, we have organized a workshop at OCWC Global 2013 "Advanced Methods and Tools for Web-Based Education".

In 2013, we were very actively involved in submitting new project proposals, particularly within the 7th Framework Programme. Once again, we were very successful in this, obtaining funding for three new projects: Proasense, Symphony and XLime. We continued with our successful efforts to include the Figure 3: iDiversiNews iPad application visualizing live stream of news Slovenian industry into the European research area; the list of 16 companies articles filtered by topic, sentiment and geographical location. participating in EU projects has been extended by two.

EU commissi s nerves 'snap' on Ukraine 16. dec. 2013 08:45 16. de arv per Your Settings Top News Items FIL st

Some outstanding publications in the past year

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- Chazal, F., Guibas, Leonidas J., Oudot, S., Škraba, P.: Persistence-based clustering in riemannian manifolds. 2. Journal of the ACM, December 2013
- Tomašev, N., Mladenić, D.: Class imbalance and the curse of minority hubs. Knowledge-based systems, 2013 3.

- 4. Anderson, A., Huttenlocher, Daniel P., Kleinberg, J., Leskovec, J.: Steering user behavior with badges. In 22nd World Wide Web Conference, *WWW-2013*, May 2013, 95–106
- Kenda, K., Fortuna, C., Moraru, A., Mladenić, D., Fortuna, B., Grobelnik, M.: Mashups for the web of things. In: ENDRES-NIGGEMEYER, Brigitte (ed.). Semantic mashups : intelligent reuse of web resources, 2013, 45–169, Berlin; Heidelberg: Springer

Organization of conferences, congresses and meetings

- 1. First International Ljubljana-Zagreb Workshop on Artificial Intelligence, Jeruzalem, Slovenia, 3.-5. 6. 2013
- 2. Conference on Data Mining and Data Warehouses, Ljubljana, Slovenia, 8. 10. 2013

INTERNATIONAL PROJECTS

- 1. 7FP PASCAL2; Pattern Analysis, Statistical Modelling and Computational Learning 2 European Commission Prof. Dunja Mladenić
- 2. 7FP MetaNET; Technologies for the Multilingual European Information Society European Commission
- Marko Grobelnik 3. 7FP - RENDER; Reflecting Knowledge Diversity European Commission
- Prof. Dunja Mladenić 4. 7FP – PlanetData
- European Commission Marko Grobelnik
- 7FP ALERT; Active Support and Real-time Coordination based on Event Processing in Open Source Software Development European Commission
- Prof. Dunja Mladenić
- 7FP SIS CATALYST; Children as Change Agents for the Future of Science in Society European Commission Prof. Dunia Mladenić
- 7FP transLectures; Transcription and Translation of Video Lectures European Commission Prof. Dunia Mladenić
- Prof. Dunja Miadeliić
 7FP LT-Web; Language Technology in the Web European Commission
- Prof. Dunja Mladenić
- 7FP Sophocles; Self-Organised information PrOcessing, CriticaLity and Emergence in multilevel Systems
- European Commission Marko Grobelnik
- 7FP MEDIAMIXER; Community Set-up and Networking for the Remixing of Online Media Fragments
 - European Commission Marko Grobelnik
- 7FP MobiS: Personalized Mobility Services for Energy Efficiency and Security through Advanced Artificial Intelligence Techniques European Commission
 - Marko Grobelnik
- 12. 7FP ProaSense; The Proactive Sensing Enterprise
- European Commission Marko Grobelnik
- 7FP SYMPHONY; Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy European Commission Prof. Dunja Mladenić
- 7FP xLiMe; CrossLingual CrossMedia Knowledge Extraction European Commission Marko Grobelnik
- 7FP X-Like; Cross-lingual Knowledge Extraction European Commission Marko Grobelnik
- 7FP TOPOSYS; Topological Complex System European Commission Dr. Primož Škraba

VISITORS FROM ABROAD

- 1. Ramesh Viswanathan, Siemens, Bengaluru, India, 3.-5. 1. 2013
- 2. Boštjan Špetič, Zemanta, New York, USA, 16. 1. 2013
- Yannis Charalabidis, University of Aegean, Athens, Greece, 22. 1. 2013
 Rachel Jones, Instrata Ltd., London, UK, 3.-6. 2. 2013
- Rudi Studer, Maria Maleshkova, Fabian Floeck, KIT, Karlsruhe, Germany, 3.–6. 2. 2013

- 7FP NRG4CAST; Energy Forecasting European Commission Maia Škrianc, B. Sc.
- PARSEME: PARSing and Multi-Word Expressions. Towards Linguistic Precision and Computational Efficiency in Natural Language Processing. COST Office
- Dr. Simon Krek
- IS1305, European Network of E-Lexicography (ENeL) COST Office Dr. Simon Krek

RESEARCH PROGRAM

1. Knowledge Technologies Prof. Dunja Mladenić

R&D GRANTS AND CONTRACTS

- Information-Communication Technologies and Transformation of Survey Research in Social Sciences Marko Grobelnik
- Model for Domain-Specific Trend Prediction based on Semantic Enrichment of Unstructured Patterns Prof. Dunia Mladenić
- Quality of Service and Quality of Experience Measurement and Control System in Multimedia Communications Environments Marko Grobelnik
- Co-authorship Networks of Slovenian Scholars: Theoretical Analysis and Visualization User Interface Development
 - Prof. Dunja Mladenić
- . Slovene Research Atlas Prof. Dunja Mladenić
- Open Communication Platform for Service Integration: CC OPCOMM Prof. Dunja Mladenić
- 7. Cloud Assisted Services: CC CLASS Marko Grobelnik
- 8. Comunication in Slovenian Language Dr. Simon Krek

NEW CONTRACTS

- Development Project for Establishing a Platform of Advanced Services for Energy Management of Household Consumers Solvera Lynx, d. d. Marko Grobelnik
- Technologies for Next-generation Intelligent Motorhome Adria Mobil, d. o. o., Novo mesto Marko Grobelnik
- 6. Abhijit Bhole, Microsoft research India, New Delhi, India, 13. 2. 2013
- 7. Maks Ovsjanikov, Ecole Polytechnique, Paris, France, 25. 2.-3. 3. 2013
- 8. Michael Witbrock, Cycorp Europe d.o.o., Ljubljana, Slovenia, 24.-27. 2. 2013, 19.-23. 6. 2013
- 9. Abraham Hsuan, Irwin & Hsuan LLC, New York, USA, 25.-30. 3. 2013, 2.-9. 10. 2013
- 10. Mark Jarecke, Elizabeth Stafford, Mike Lee, FOUR32C, New York, USA, 23.-30. 3. 2013
- 11. Marko Tadić, University of Zagreb, Zagreb, Croatia, 25.–26. 3. 2013
- 12. Kiyoshi Nitta, Yahoo! Research, Tokio, Japan, 29. 4. 2013
- 13. Božidar Kliček, Faculty of Organization and Informatics, Varaždin, Croatia, 10. 6. 2013

- 14. Dijana Oreški, Faculty of Organization and Informatics, Varaždin, Croatia, 11. 6. 2013
- 15. Alek Kolcz, Twitter, San Francisco, USA, 20.-23. 6. 2013
- 16. Danica Kragić, KTH, Stockholm, Sweden, 1.-4. 6. 2013
- 17. Ulrich Bauer, Hubert Wagner, IST Austria, Klosterneuburg, Austria, 1.-4. 7. 2013
- 18. Mateusz Juda, Jagiellonian University, Krakow, Poland, 1.-4. 7. 2013
- 19. Florian Pokorny, KTH, Stockholm, Sweden, 1.-4. 7. 2013
- 20. Calin Railean, Technical University Cluj-Napoca, Cluj-Napoca, Romania, 1.-15. 9. 2013
- 21. Frank van Harmelen, VU Amsterdam, Amsterdam, Netherlands, 27. 6.-7. 7. 2013

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- Asst. Prof. Iztok Savnik 5
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- 14. Dr. Inna Novalija
- 15. Dr. Joao Paulo Pita Da Costa
- 16. Dr. Polona Škraba Stanič
- 17. Dr. Mikael Vilhelm Vejdemo Johansson

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- 18. Luka Bradeško, B. Sc.
- 19. Rayid Ghani, M. Sc. 20. Deian Gove"
- 21. Mitja Jermol, M. Sc.

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- 22. Lynd Hratman, CWI Amsterdam, Amsterdam, Netherlands, 28. 6.-7. 7. 2013
- 23. Rok Sosič, Stanford University, Palo Alto, USA, 23. 8. 2013
- 24. Christopher Stone, Harvey Mudd College, Claremont, USA, 19. 9. 2013
- 25. Olegas Niksou, Vilnius University, Vilnius, Lithuania, 7.-8. 10. 2013
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- 28. Mirjana Ivanović, Miloš Radovanović, University of Novi Sad, Novi Sad, Serbia, 17.-19. 11. 2013
- 22. Blaž Kažič, B. Sc.
- 23. Dr. Aljaž Košmerlj
- 24. Blaž Novak, B. Sc. 25. Jan Rupnik, B. Sc.
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- 31. Mojca Mikac, B. Sc.
- 32. Matjaž Rihtar, B. Sc.
- 33. Klemen Simonič, B. Sc., left 17.08.13
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- 39. Mateja Zver, B. Sc.

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INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

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SCIENTIFIC MONOGRAPH

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MENTORING

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 Carolina Fortuna, Dynamic composition of communication services: doctoral dissertation, Ljubljana, 2013 (mentor Mihael Mohorčič; co-mentor Dunja Mladenić)
- mentor Dunja Mladenić).
- 3. Nenad Tomašev, The role of hubness in high-dimensional data analysis: doctoral dissertation, Ljubljana, 2013 (mentor Dunja Mladenić).
- Domen Šoberl, Distributed computation of homology in wireless sensor networks: master's thesis, Ljubljana, 2013 (mentor Neža Mramor-Kosta; co-mentor Primož Škraba).

LABORATORY FOR OPEN SYSTEMS AND NETWORKS E-5

The main activities of the laboratory are the R&D of next-generation networks, telecommunications technologies, components and integrated systems and information-society services and applications, especially those that ensure an efficient and pervasive life-long learning concept.

In 2013 the research group implemented the research program "Future Internet Technologies: concepts, architectures, services and socio-economic issues". Research was also carried out in the EU 7FP project "UNITE", the "STORK 2.0" and "eSENS" projects from the CIP programme, the "SELPRAF" project from the Leonardo da Vinci programme, the "Twin Tide" project from the COST programme, and in a few national projects. The main fields of work were technologies and services in advanced, next-generation networks, security and privacy in information systems, and technology-enhanced learning. Members of the laboratory are also teaching at the undergraduate and graduate levels at the University of Ljubljana, the Jožef Stefan International Postgraduate School, and the DOBA Faculty. In 2013 they were mentors at two master theses and one diploma thesis.



Prof. Borka Jerman Blažič

Concepts, architectures, technologies and services in the future internet

In the area of the Future Internet we successfully finished the "Upgrading ICT excellence by strengthening the cooperation between research Teams in an enlarged Europe (UNITE)" project. The main goals of the project were the organization of researchers and PhD students exchange between EU research, academic and industrial

organizations, the organization of targeted workshops, such as doctoral symposiums, across an enlarged Europe to build-up synergies and support networking and collaboration, and the creation of virtual communities for the institutions involved in research of the Future Internet.

Among our most important R&D results in this area in 2013 is a Future Internet collaboration platform that supports a number of advanced synchronous and asynchronous collaboration activities and services, e.g., multimedia-based communication, public/private chat, screen sharing, voting, recording, skills and competencies-based content tagging, efficient P2P-based content distribution, and authentication with standard e-identity credentials or graphical passwords on mobile devices. The platform's building blocks are based on open-source technologies, such as OpenMeetings and Matterhorn, and the technologies we developed in collaboration with other partners in a number of EU projects, such as P2P-Next (NextShare), OpenScout or STORK. The platform has been successfully tested in a commercial environment.



Figure 1: Future collaboration platform

Technology-enhanced learning

The general aim of the successfully finished Leonardo da Vinci LLP "Self-employment with e-learning based Practice Firms (SELPRAF)" project was to encourage people's interest in entrepreneurship through an innovative SELPRAF Training Programme for the acquisition of the four key competences (communication in the mother tongue, communication in foreign languages, digital competence, and sense of initiative and entrepreneurship) and, on the other hand, to enable the inclusion of the unemployed in practice firms and to encourage self-employment. In 2013 we conducted a pilot SELPRAF training, which was attended by 227 unemployed people in Slovenia and Croatia. They have carried out more than 4,500 hours of distance learning and the top 48 trainees were later included in the practice firms where they trained real business. According to the very positive feedback from the trainees, the innovative educational program SELPRAF, based on know-how and the transfer of practical experience, can achieve already in the medium-term perspective more stimulating working environment and stronger interest for entrepreneurship.

The main objective of the COST project "Towards the Integration of Transectorial IT Design and Evaluation (Twin-Tide)" that also ended in 2013 was to harmonize and integrate research findings and achievements with practice during the process of designing and evaluating information technologies across various sectors and disciplines. In November 2013 we co-organized in Bled an international TwinTide autumn training school **TUTOREM**'2013 for PhD students from the HCI field. The overarching goal of TUTOREM was to improve the participants' understanding of significant research methods commonly or increasingly used in the field of HCI. Such an enhanced understanding will enable them to select and combine appropriate research methods for their specific HCI projects and to contex-



Figure 2: TUTOREM school for Ph.D. students

tualise them without unintended impacts on validity. The TUTOREM School was attended by 32 PhD students and 7 professors from all over Europe.

In 2013 we successfully finished two bilateral scientific cooperation projects: the first one with the Republic of Cyprus in the field of creative information spaces for problem-based learning and the second one with the Republic of Serbia within the scope of applications of workflow management technology in e-learning systems. The results of the joint research have already been published in a scientific journal with an SCI impact factor and at three international conferences. Furthermore, we continued with the analysis of business games suitable for e-learning and education and presented the results at two conferences.

We were also successful in obtaining new projects from the EU's 7FP. "Scalable cost-effective facilitation of professional identity transformation in public employment services (EmployID)" was the highest ranked project proposal among more than 100 proposals in the whole field of technology enhanced learning. The main goal of the project that will start in February

2014 is to support and facilitate the learning process of PES (Public Employment Services) practitioners in their professional identity development by the efficient use of technologies to provide advanced coaching, reflection, networking and learning support services.

Security, dependability and privacy in information systems

The provision of security and privacy services is crucial for the modern information society. In 2013 our activities in this field were focused on R&D in security context-aware mechanisms and services for advanced systems and networks, such as pervasive systems, e-identity-based services, trust and reputation management, cloud computing security, and security economics.

Ubiquitous social systems impose several challenges with respect to traditional security. A security system applicable for such environments should enable open interaction between entities and devices and protect resources in proportion to their importance and according to the security context. We proposed a conceptual model of security context that takes into account related social aspects and defines a set of concepts at the appropriate level of abstraction. The model promises to facilitate the specification, management and reuse of security policies in complex and dynamic environments.

Online trust systems aim to translate the role that trust has in the traditional world onto network-based systems. In a scientific paper in a journal with an SCI impact factor we determined the systemic features of trust and introduced a novel framework of design properties. We described the systemic properties that lack in the current technical solutions, and incorporated social factors into the design guidelines of trust systems. This paper is the first study applying fundamental social science principles from General Systems Theory and case-study research for the purpose of theory building and the evaluation of technical human-centric solutions.

The Laboratory for Open Systems and networks is a member of two large-scale pilot projects, STORK and eSENS, that are developing a pan-European infrastructure for cross-border e-services. The goal of a "Secure identity across borders linked 2.0 (STORK 2.0)" project with 58 partners from 19 European countries is to enable e-identity-based services across borders in the fields of e-academia, e-banking, public services for business, and e-health. The project that started in 2012 will demonstrate interoperable services in real-life settings and validate common specifications, standards and building blocks, exploring scenarios to address challenging legal and governance issues (across borders, application domains and different sectors) decisively pushing the lines for the wider uptake of eID in Europe. Our main activities in 2013 included setting up a common infrastructure on a European level and the implementation of three e-academia services, in particular a virtual learning environment, an anonymous electronic survey service, and a job-selection service. The "Electronic Simple European Networked Services (eSENS)" project that started in 2013 will consolidate the building blocks of the existing large-scale pilots, including STORK 2.0, focusing strongly on the core building blocks such as eID, eDocuments, e-Delivery, and e-Signatures. Our laboratory is leading project activities on user attributes provision and aggregation and role management.

Electronic identity-related research activities were also part of the "Cloud assisted services (CLASS)" project. The centre connects a number of Slovenian companies, universities and research institutions with an aim to develop services and products in the area of cloud computing. The most important result of our activities in 2013 is a proto-type of a single sign-on solution that works across a variety of cloud platforms (OpenStack, VMware). The solution

enables the reduction of certain security risks, while providing the possibility of the centralised control of users. It has already been well received among the open-source developers and companies in the field of cloud computing.

In the area of security-related research activities we continued with research on security economics, where we analyse the assessment of the appropriate investment that is economically affordable and provides enough protection for enterprise information systems. The result, i.e., an updated approach to the quantification of the necessary investment and a recommendation for a standard approach to security-information investment assessment, has been published in a scientific journal "Engineering management journal" with an SCI impact factor.

The laboratory was very successful in 2013 in obtaining new EU projects from 7FP and the ISEC programme also in the security field. The main goal of the COURAGE, REDIRNET and DFET projects is to deliver a research agenda for cyber crime and cyber terrorism, provide a decentralized framework for interoperability for first responders' systems, and develop a cloud-based cybercrime and forensics training and evaluation environment. All three projects will start with their activities at the beginning of 2014.

Science promotion

In September 2013 the Laboratory for Open Systems and Networks successfully organized Researcher's Night 2013 with the goal to promote science, scientists and their results. The event was organized in collaboration with Faculty of Information Studies Novo mesto and the National Institute of Biology within the 7FP "REsearchers for NAture preservation and TECHnology use for the benefit of the society (RENATECH)" project. "Researchers contributing to the nature preservation and the technology applications for the benefit of the society" was the major focus of the Researcher's Night 2013 in Slovenia. In order to reach the specific objective of bringing researchers closer to the public at large the Researcher's Night was organized at different locations in Ljubljana (Congress Square, National Institute of Biology, Šentvid High School, Ljubljansko barje Landscape Park), Novo mesto (Faculty of Information Studies) and Piran (Marine Biology Station). The event was widely recognized by the broader society, which proved that there is definitely a lack of projects and events with similar contents and that scientists are keen to share their experience with their colleagues and in this way stimulate the



Figure 3: Researchers' Night 2013

young who are just at the beginning of their careers. The estimated total number of visitors at all venues was around 6000. The event received great attention in national media (national TV and radio, POP TV, etc.).

Some outstanding publications in the past three years

- 1. Bojanc, R., Jerman-Blažič, B., Tekavčič, M.: Managing the investment in information security technology by use of a quantitative modeling. *Inf. process. manage.*, 2012, vol. 48, no. 6, 1031–1052
- Jerman-Blažič, B.: Four scenarios for future evolution of the internet. IEEE technology & society magazine, ISSN 0278-0097, 2011, vol. 30, no. 4, 39-46
- 3. Mihajlov, M., Jerman–Blažič, B.: On designing usable and secure recognition-based graphical authentication mechanisms. Interact. comput.. [Print ed.], 2011, vol. 23, no. 6, 582–593

Organization of conferences, congresses and meetings

- 1. The 2013 Researchers' Night, RENATECH Project, 27. 9. 2013
- 2. Organisation of "TwinTide" Training School, Bled, Slovenia, 4.-8. 11. 2013

INTERNATIONAL PROJECTS

- 1. 7FP UNITE; Upgrading ICT Excellence by Strengthening Cooperation between Research Teams in an Enlarged Europe European Commission
- Prof. Borka Džonova Jerman Blažič
 7FP ReNATECH; REsearchers for NAture preservation and TECHnology use for the benefit of the society
 European Commission
 - Prof. Borka Džonova Jerman Blažič
- 3. STORK 2.0; Secure idenTity acrOss boRders LinKed 2.0 European Commission
 - Prof. Borka Džonova Jerman Blažič

- CIP-e-SENS; Electronic Simple European Networked Services European Commission Prof. Borka Džonova Jerman Blažič
- COST IC0904; Towards the Integration of Trans-sectorial IT Design and Evaluation COST Office Matija Pipan, M. Sc.
- G. Creative Multimodal Information Spaces for Problem-based Learning Slovenian Research Agency Asst. Prof. Tanja Arh
- Application of Workflow Management Technology in E-learning Systems Slovenian Research Agency Asst. Prof. Tanja Arh

RESEARCH PROGRAM

 Future Internet Technologies: Concepts, Architectures, Services and Socio-Economic Issues Prof. Borka Džonova Jerman Blažič

R&D GRANTS AND CONTRACTS

- 1. Future Internet Collaboration Platform
- Prof. Borka Džonova Jerman Blažič 2. Cloud Assisted Services: CC CLASS
- . Cloud Assisted Services: CC CLASS Prof. Borka Džonova Jerman Blažič

8 Maks Mržek B Sc

10. Matija Pipan, M. Sc.

12. Tatjana Martun, B. Sc

* part-time JSI member

11. Svetlana Sapelova

9

Note:

Tanja Pavleska, B. Sc.

Technical and administrative staff

3. LdV - SELPRAF; Self-employment with e-Learning based Practise Firms Asst. Prof. Tanja Arh

VISITORS FROM ABROAD

1. Dr. Andri Ioannou, Prof. Dr. Panayiotis Zaphiris, Christina Vasiliou, Cyprus University of Technology, CUT, Limassol, Cyprus, 17.-20. 10. 2013

STAFF

Researchers

- 1. Asst. Prof. Tanja Arh
- 2. Asst. Prof. Rok Bojanc*
- 3. Prof. Borka Džonova Jerman Blažič, Head
- 4. Asst. Prof. Tomaž Klobučar

Postdoctoral associate 5. Dr. Dušan Gabrijelčič

Postgraduates

- 6. Andrej Jerman Blažič, M. Sc.
- 7. Vladimir Jovanovikj, B. Sc.

BIBLIOGRAPHY

ORIGINAL ARTICLE

- 1. Tanja Ažderska, Borka Jerman-Blažič, "A holistic approach for designing human-centric trust systems", *Syst. pract. action res. (Dordr., Online)*, vol. 26, no. 5, pp. 417-450, 2013.
- Rok Bojanc, Borka Jerman-Blažič, "A quantitative model for information-security risk management", *Eng. manag. j.*, vol. 25, no. 3, pp. 25-37, 2013.

REVIEW ARTICLE

1. Tomaž Klobučar, "Sodobne e-izobraževalne tehnologije", *Mednarodno inovativno poslovanje*, vol. 5, no. 1, 2013.

PUBLISHED CONFERENCE CONTRIBUTION

- 1. Rok Bojanc, "Interoperabilna platforma z enotno vstopno točko", In: *Dvajset let pozneje: zbornik prispevkov*, 20. konferenca Dnevi slovenske informatike, Portorož, 15.-17. april 2013, Tomaž Gornik, ed., 1. izd., Ljubljana, Slovensko društvo Informatika, 2013, pp. 1-10.
- 2. Cormac Callanan, Borka Jerman-Blažič, Heins Dries-Ziekenheiner, "Empirical assessment of data protection and circumvention tools availability in mobile networks", In: *Proceedings*, The Second International Conference on Cyber Security, Cyber Peacefare and Digital Forensic, CyberSec2013, March 4-6, 2013, Kuala Lumpur, Kuala Lumpur, The Asia Pacific University of Technology and Innovation, 2013, pp. 206-220.
- Andrej Jerman Blažič, Tanja Arh, "Business simulation game an innovative pedagogical approach in business environment", In: *Zbornik*, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 136-141.
- 4. Andrej Jerman Blažič, Tanja Arh, "Immersive business simulation games: an innovative pedagogical approach to e-learning and education", In: *Electric dreams: proceedings*, 30th Ascilite Conference, 1-4 Secember 2013, Sydney, H. Carter, ed., M. Gosper, ed., J. Hedberg, ed., Sydney, Aacquarie University, 2013.

- Andrej Jerman Blažič, Tanja Arh, "Resne poslove igre: nov pristop k učenju projektnega menedžmenta: a new approach to project management learning", In: *Izzivi gospodarskega razvoja - inovativni* projektni management: zbornik prireditve, Ljubljana, 20. in 21. maj 2013, Ljubljana, GZS, Zbornica osrednjeslovenske regije, 2013, pp. 99-104.
- 6. Vana Kamtsiou, Tomaž Klobučar, "Integrating roadmapping and disagreement management methodologies for coordinating development of competency-driven education standards: the ICOPER Case", In: *Technology management in the IT-driven services: PICMET '13 conference,* Portland International Center for Management of Engineering and Technology, July 28 August 1, 2013, San Jose, California, USA, Portland, PICMET, 2013, pp. 2236-2247, 2013.
- Matija Pipan, Bojan Srdjević, Julija Lapuh Bele, Zorica Srdjević, "Comparison of decision making results in case of LMS selection", In: Pametna organizacija: talenti, vitka organiziranost, internet stvari: zbornik 32. mednarodne konference o razvoju organizacijskih znanosti: high potentials, lean organization, internet of things: proceedings of the 32nd International Conference on Organizational Science Development, 32. mednarodna konferenca o razvoju organizacijskih znanosti, 20.-22. 3. 2013, Portorož, Slovenija, Zvone Balantič, ed., et al, Kranj, Moderna organizacija, 2013, pp. 847-854.
- 8. Christina Vasiliou, Andri Iannou, Tanja Arh, Panayiotis Zaphiris, Tomaž Klobučar, "Technology enhanced problem based learning", In: Pametna organizacija: talenti, vitka organiziranost, internet stvari: zbornik 32. mednarodne konference o razvoju organizacijskih znanosti: high potentials, lean organization, internet of things: proceedings of the 32nd International Conference on Organizational Science Development, 32. mednarodna konferenca o razvoju organizacijskih znanosti, 20.-22. 3. 2013, Portorož, Slovenija, Zvone Balantič, ed., et al, Kranj, Moderna organizacija, 2013, pp. 1187-1195.
- Nikola Vitković, Miodrag Manić, Miroslav Trajanović, Dragan Mišić, Milorad Mitković, Tanja Arh, Matija Pipan, "eLearning system for medical education based on the geometrical models of human bones and fixators", In: *Proceedings*, eLearning 2013, The Third International Conference on e-Learning, Belgrade, September 26-27, 2013, Danijela Milošević, ed., Belgrade, Metropolitan University, 2013, pp. 10-14.
- Srečo Zakrajšek, Tanja Arh, "Kako do dobrih idej za uspešne projekte?", In: Izzivi gospodarskega razvoja - inovativni projektni management: zbornik prireditve, Ljubljana, 20. in 21. maj 2013, Ljubljana, GZS, Zbornica osrednjeslovenske regije, 2013, pp. 131-138.

MENTORING

- 1. Blaž Ivanc, Modelling of information attacks on critical infrastructure by using an enhanced structural model: master's thesis, Ljubljana, 2013 (mentor Tomaž Klobučar).
- 2. Frančiška Avbelj, Establishment of e-learning for health and safety at work: master's thesis, Maribor, 2013 (mentor Tomaž Klobučar).

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, computer simulations supporting biomedical procedures and specialised equipment and procedures for advanced bio-signal processing and interpretation.

The research and development activities at the department are carried out in the framework of the Communication Technology Laboratory (CTL), the Parallel and Distributed Systems Laboratory (PDSL) and the Networked *Embedded Systems Laboratory (NESL).* The research work of the three laboratories is complementary, which is reflected in the joint applied projects.

In 2013 the research activities within the Communication Technology Laboratory were concentrated on Head: different challenges associated with access-segment technologies, enabling end-users to access new multimedia Asst. Prof. Mihael Mohorčič services and applications. As part of the multi-year telecommunication-systems research programme the emphasis was on research in the areas of: radio propagation, access architectures for heterogeneous wireless networks,

management of radio and network resources and cognitive communications. The investigation of the radio-signal propagation was focused on two main topics. The first topic concerns the research of the radio-signal propagation in special environments, such as long road and railway tunnels. The emphasis was on the radio-signal propagation in typical frequency bands for voice communication systems (400 MHz), high-speed data communication systems (2.4 GHz and 3.5 GHz) and low-data-rate wireless sensor networks (868 MHz and 2.4 GHz). We published the research results in the paper "A survey of radio propagation modelling for tunnels", issued in the journal IEEE

Communications Surveys and Tutorials. The second topic, researched in cooperation with Telekom Slovenije d.d., concerns the development, implementation and testing of software modules for radiowave propagation modelling in mobile communication systems for rural and urban environments, including statistical channel models as well as channel models based on ray tracing and their integration into the open-source geographic information system (GIS). For the ray-tracing method we started research into efficient acceleration techniques using massively parallel

hardware and an optimization method applicable to a wider set of problems solved by SIMD processors was proposed.

We continued the investigation of advanced concepts and technologies for a capacity increase of wireless meshed networks using network coding techniques. In particular, we focused on the development of advanced network coding algorithms and their adapted routing procedures. In order to support the performance evaluation of arbitrary network-coding algorithms on predetermined or randomly generated topologies of wireless meshed networks, we designed and built a simulation model, which allows the performance evaluation of network coding algorithms and routing procedures on randomly generated wireless mesh network topologies.

In collaboration with European partners within the FP7 ABSOLUTE project (Aerial Base Stations with Opportunistic Links for Unexpected & Temporary Events) we participated in the design and validation of an innovative, rapidly deployable future network architecture. It should be resilient Figure 1: Air-quality monitor based on the VESNA platform. and capable of providing broadband multi-service, secure and dependable connectivity for large coverage areas affected by large-scale unexpected events (or disasters) leading to the partial or complete unavailability of the terrestrial communication infrastructure, or for temporary events requiring very high throughput and augmented network capacity. We focused on the

For integration into the open-source geographic information systems GRASS, we developed and implemented a software module for the radio-wave-propagation modelling in mobile communication systems based on ray tracing.

We designed and developed new hardware and software modules and implemented new features for the VESNA platform.



For the needs of different projects we expanded the sensor network-based testbed LOG-a-TEC, supporting experimental research in radio and networking areas and in the Internet of Things applications.



Figure 2: Alphasat satellite receiver, developed at the JSI and installed in collaboration with the Joanneum Research Institute on the Hilmwarte tower in Graz, Austria.

development of new advanced techniques for radio-spectrum management, on the development of new network solutions and on the integration of wireless sensor networks into the emergency architecture.

In 2013 we were actively participating in several COST actions. In the COST Action IC0902 "Cognitive Radio and Networking for Cooperative Coexistence of Heterogeneous Wireless Networks" we presented an original method for calculating the radio environment map and compared it with

selected existing methods. With an independent chapter on low-cost experimental networks for prototyping solutions in the field of cognitive radio, we contributed to a book that will be published in 2014 by Springer. In the COST Action IC1101 "Optical Wireless Communications An Emerging Technology" we investigated in cooperation with TU Graz the influence of weather conditions on the performance of wireless optical communication systems. In the COST Action IC1104 "Random Network Coding and Designs over GF(q)", we are developing practical network coding procedures and evaluating them in a purpose-built simulation model. In the COST action IC1004 "Cooperative Radio Communications for Green Smart Environments" we mainly participate in working groups one and two, with topics related to radio propagation aspects and problems of the physical layer.

In the ESA PECS project SatProSi we developed a low-cost SDR-based ground station for reception of the Ka-band satellite signals from EUTELSAT HotBird 6, SES ASTRA 3B and joint ESA and Inmarsat Alphasat satellite, which is intended for long-term monitoring of the satellite carrier and modelling of the satellite channel. Software tools were also developed for a statistical analysis of the received signal data.

In the area of cognitive communications we continued research in the radio and access segments and contributed to the WUN-CogCom and FP7 CREW projects. In 2013 our research in this area was focused on stand-alone and collaborative spectrum sensing in licensed and unlicensed frequency bands and on building radio environmental maps.

In cooperation with the Department of Low and Medium Energy Physics (F2) we continued research activities that were started in previous years which were focused primarily on efficient signal-processing algorithms in high-count-rate gamma-ray spectrometry.

In the **Parallel and Distributed Systems Laboratory**, we successfully continued interdisciplinary research work in the framework of the program group that also includes the Machine Vision Laboratory from the Faculty of Electrical Engineering and the Laboratory for Algorithms and Data Structures from the Faculty of Computer and Information Science, both from the University of Ljubljana. We were heavily involved in research within the research program Parallel and Distributed Computing and also in other research projects. Our cooperating researchers also come from industry (Turboinstitut d.d. and Xlab d.o.o.) and from the medical sphere (the University Clinical Center Ljubljana).

In the frame of the EU FP7 CREW project and the FIRE initiative the LOG-a-TEC testbed is used as a real-world outdoor experimental environment for the cognitive radio and cognitive networking research.



Figure 3: Radio signal coverage calculation using the in-housedeveloped radio coverage tool GRASS RaPlaT

We investigated computer algorithms for efficient implementation on parallel and distributed computers, testing them on a research computer cluster that is stationed in our department facilities, and on a cloud recently installed in cooperation with the Faculty of Computer and Information Science of the Ljubljana University and Turboinstitut d.d. In addition to demanding computations, we also paid attention to distributed large data storage. We continued investigations in the field of wireless sensor networks based on the theory of parallel and distributed computing and communication.

We developed new parallel numerical algorithms, e.g., meshless methods, which are local and, hence, efficiently executable on parallel computers. With these methods we can simulate physical phenomena, e.g., heat and fluid flows, PN junctions and molecular dynamics in realistic conditions. We developed software for simulating biological systems, e.g., lipid membranes and biomedical procedures, such as post-surgical cryotherapy and RF, and cryo-ablation of the heart. We parallelized multi-criterion optimizations and began to investigate how to efficiently integrate measurement results, simulation results and optimization methods, which will enable us to predict biological parameters that are hard to measure in a non-invasive manner.

We evaluated a new methodology for synthesising the standard ECG from a small number of differential measurements. We investigated possible options for an analysis of large signal sets with the human auditory system

(sonification). We investigated possible options for the detection of respiratory sinus arrhythmia (RSA) in the ST interval. We developed a new method for measuring the variability of the ST interval with a sub-millisecond resolution. Together with neurologists from the University Clinical Center Ljubljana, we continued equipment upgrading and measurements for the NeuroECG.

In the area of cardiology we have fortuitously documented a spontaneous cardio-inhibitory syncope using a high-precision 31-channel body-surface ECG measurement, which is probably a unique measurement of this type. Detailed analysis of the atrial activity (P waves) in this recording has shown that a functional pacemaker area exists outside the sinoatrial node. The activity of this area emerged with a profound influence of the autonomic nervous system on the sinoatrial node. After a few heart beats the activity of this area ceased causing the syncope.

We collaborated with the Laboratory for Molecular Modelling at the National Institute of Chemistry, and parallelized and consequently significantly speeded up their web service ProBiS. We then continued the successful collaboration by developing a new parallel algorithm for finding the maximum clique in undirected graphs. Finding the maximum clique in a graph is a NP-full problem, which is an important sub-problem in the problem of finding similarities between molecules.

In a project sponsored by the Marine Biological Station (MBP) from Piran we parallelized the software package NAPOM (North Adriatic Princeton Ocean Model). NAPOM represents the central part of the prognostic software system for the north Adriatic Sea. Its parallelization is the first step towards its modernization, through which MBP wishes to increase the model resolution and thus increase the prognostic capabilities on the Slovenian part of the Adriatic Sea.

In the field of formal methods for discrete systems development, we investigated the synthesis, also such with global optimization, of complete test suites for final state machines, also for the needs of distributed testing, for non-standard conformance relations and for non-standard assumptions about the properties of the automaton under test.

In 2013 the Networked Embedded Systems Laboratory mainly focused on research and development in the areas of the Internet of Things and cognitive communications. The emphasis was on the vertical integration of different wireless sensor and communication network technologies with semantic technologies in support of the autonomous search and composition of sensors and sensor data, as well as on the development of new applications using various machine-learning and decision-making algorithms. These activities were mainly conducted within the basic research

project "Advanced procedures for interactive composition of sensor networks" and the EU FP7 Network of Excellence PlanetData.

The modular and fully flexible platform VESNA for wireless sensor networks, developed as the core building block for several research and applied projects, was complemented with a set of new modules and new features in existing modules, including radio spectrum sensing in the UHF

We compared the calculation complexities of different meshless methods for solving a diffusion equation and concluded that strong formulated approaches are computationally more efficient than weak formulations.



Figure 4: Body surface 31-channel ECG recording shows electrical activity (P waves) of the atria just before the emergency of spontaneous cardioinhibitory syncope (upper panel). Colour presentation of the electrical potential on the body surface, 10 ms after the start of the activity in the atria (lower panel). The positions of the electrodes are denoted by small circles.

We developed a prototype wireless electrode of bio-potentials from the body surface for the concurrent measurements of the ECG and the respiration rate.

and ISM frequency bands within the EU FP7 CREW project, a suite of motion, location, presence and ambient sensors within the national competence centre KC OpComm, a framework for the semantic description of sensor node functionalities and status, wired and wireless gateway capabilities for internet connectivity or interaction with other devices, etc. A variety of supported features, protocols and technologies, together with an arbitrary combination of developed hardware and software modules, make the VESNA platform well suited for the implementation of an experimental research sensor networks infrastructure, the deployment of pilot applications, the validation of usage scenarios and the development of end-user solutions.



Figure 5: In-vivo measurements of average temperatures of all patients during cooling treatment in Group A with the gel-pack (left) and Group B with the cTreatment® (right). Abbreviations: ICN- intercondylar notch, SCsubcutaneous, SK-skin (12 - anterior, 3 - medial, 6 - posterior, 9 - lateral), BA - bandage.

We synthesised, with a high reliability, a standard 12-lead ECG from three bipolar wireless electrodes.

In collaboration with the Municipality of Logatec and Komunalno podjetje Logatec we upgraded a large-scale outdoor wireless sensor network LOG-a-TEC experimental testbed. The testbed is based on the VESNA platform and equipped with a set of sensors and communication interfaces, as required by a given project. The sensor nodes' firmware management,

the execution of experiments and the gathering of sensor measurements data is performed via a web application running on one of our servers. In the current setup built for the FP7 CREW project the LOG-a-TEC testbed consists of more than 50 nodes in two clusters and allows the execution of experimentally-driven research in the areas of spectrum sensing in licensed and unlicensed frequency bands, cognitive radio and cognitive networking. As a part of the CREW testbeds federation this part of LOG-a-TEC also represents one of the FIRE facilities, i.e., the only one supporting the investigation of horizontal and vertical radio-spectrum-sharing methods in a real-world outdoor



Figure 6: Results of a numerical simulation of binary material solidification (Sn-10%Pb) (left) where the concentration and velocity fields are presented at the moment when instabilities appear and the simulation of the PN junction, where the density distribution of electric carriers in a semiconductor device is presented.

environment and being particularly well suited for experiments in TV white spaces. The LOG-a-TEC testbed has been complemented with another location at the JSI, where VESNA platforms are equipped with Contiki OS and intended for experimentation with cognitive networking on MAC and higher layers using the ProtoStack tool for remote composition, reconfiguration and reprogramming of the CRime protocol stack.

Our research work in the frame of the national competence centre KC OpComm, aiming at the development of an open communication platform for the development of new types of services and applications for the Future Internet, was concentrated on the provision of data and context information from sensor networks to management services and applications. To this end, we continued developing different VESNA platform modules, investigating procedures for the pre-processing of data and metadata, and developing the required communication protocols and interfaces for the platform. Related

to these activities we developed sensoric support for an asset-management application and remote monitoring of the photovoltaic power plant at Telekom Slovenije.

In the area of remote monitoring we continued the work in the EU FP7 project BalkanGEONet concerned with the inclusion of all Balkan countries into GEO. In the area of wireless sensor networks we continued two FP7 projects. In the ABSOLUTE project our role is to integrate a VESNA-based wireless sensor network in the emergency communications network architecture. The aim is to provide easily deployable sensor network for in-situ fixed or participatory monitoring of post-disaster parameters as well as for the spectrum sensing needed to support the ad-hoc establishment of the ABSOLUTE communication system without causing harmful interference to coexisting communication systems. In the CITI-SENSE project, which is concerned with the establishment of sensor-based Citizens' Observatory Community for improving the quality of life in cities, our focus was mainly on providing the

- We fortuitously documented a unique measurement of spontaneous cardioinhibitory syncope by high-precision 31-channel body-surface ECG.
- We parallelized and thus speeded up two software packages that are in active use, one in the Marine Biological Station and one in the National Institute of Chemistry.
- We improved a simulation model for the performance evaluation of network-coding techniques.

VESNA-based solution for air-quality monitoring. As part of this we were developing modules with gas, particle matter and other ambient related sensors, which would be used for indoor and outdoor environment monitoring.

In 2013, we started two technology development projects financed by the Ministry of Economic Development and Technology, namely "Smart camper" and "Smart home". In the first one, in collaboration with the company Adria Mobil, we started developing sensor and communication technologies for the intelligent remote management of motorhomes. In the second project, together with the company Cosylab, we started developing sensor and communication technologies for smart buildings, with an emphasis on monitoring the generation and consumption of electricity.

The Networked Embedded Systems Laboratory and its research and development activities also take part in the SensorLab group, which was established by the Department of Communication Systems and the Laboratory of Artificial Intelligence.

Some outstanding publications in the past year:

- Hrovat, A., Kandus, G., Javornik, T.: A survey of radio propagation modeling for tunnels. IEEE Communications surveys and tutorials, 2013, 12 pgs., doi: 10.1109/SURV.2013.091213.00175
- Volkov, A., Žganec Gros, J., Žganec, M., Javornik, T., Švigelj, A.: Modulated acquisition of spatial distortion maps. Sensors, ISSN 1424-8220, 2013, vol. 13, no. 8, 11069–11084, doi: 10.3390/s130811069

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- 4. Kosec, G., Zinterhof, P.: Local strong form meshless method on multiple Graphics Processing Units. CMES-Comp Model Eng. 2013;91:377–96
- 5. Kosec, G., Šarler, B.: Solution of a low Prandtl number natural convection benchmark by a local meshless method. Int J Numer Method H. 2013;23:22
- 6. Avbelj, V., Trobec, R.: A closer look at electrocardiographic P waves before and during spontaneous cardioinhibitory syncope: letter to the editor. Int. j. cardiol., 166 (2013) 3, e59–e61.
- Rashkovska, A., Trobec, R., Avbelj, V., Veselko, M.: Knee temperatures measured in vivo after arthroscopic ACL reconstruction followed by cryotherapy with gel-packs or computer controlled heat extraction, Knee Surg Sports Traumatol Arthrosc, early publ. doi:10.1007/s00167-013-2605-x, 2013

Awards and appointments

1. Aleksandra Rashkovska: Special prize for innovations for economy at the 6th International Transfer Conference and Innovation Day 2013, Brdo pri Kranju, Slovenia, Smart Thermo Therapy

Patents granted

- Bojan Likar, Robert Posel, Andreas Kalagasidis, Tomaž Javornik, Gorazd Kandus, Mihael Mohorčič, Aleš Švigelj, Janez Bešter, Andrej Kos, Miha Smolnikar, Iterative localization techniques, US8565106 (B2), US Patent Office, 22.10.2013.
- Bojan Likar, Robert Posel, Andreas Kalagasidis, Tomaž Javornik, Gorazd Kandus, Janez Sterle, Urban Sedlar, Janez Bešter, Andrej Kos, Luka Mali, Method for self organizing network operation, US8472334 (B2), US Patent Office, 25.6.2013.

INTERNATIONAL PROJECTS

- 1. 7FP PlanetData European Commission
 - Asst. Prof. Mihael Mohorčič
- 7FP BalkanGEONet; Balkan GEO Network-Towards Inclusion of Balkan Countries into Global Earth Observation Initiatives European Commission
- Asst. Prof. Mihael Mohorčič
- 3. 7FP CREW; Cognitive Radio Experimentation World European Commission
- Asst. Prof. Mihael Mohorčič
- 7FP ABSOLUTE; Aerial Base Stations with Opportunistic Links for Unexpected & Temporary Events European Commission
- Asst. Prof. Mihael Mohorčič
- 7FP CITI-SENSE; Development of Sensor-based Citizens' Observatory Community for Improving Quality of Life in Cities European Commission
- Asst. Prof. Mihael Mohorčič 6. 7FP - VHP NoE; Virtual Physiological Human Network of Excellence European Commission
- Prof. Roman Trobec
- 7. ESA PECS; Processing of Satellite Signals in Ka/Q-frequency Band ESA/ESTEC.
- Prof. Gorazd Kandus
- 8. COST IC1004; Cooperative Radio Communications for Green Smart Environments COST Office
- Asst. Prof. Tomaž Javornik 9. COST IC1101; Optical Wireless Communications - An Emerging Technology
- COST Office
- Prof. Gorazd Kandus
- COST IC0906; WiNeMO; Wireless Networking for Moving Objects COST Office Miha Smolnikar, B. Sc.
- 11. COST ICO902; Cognitive Radio and Networking for Cooperative Coexistence of Heterogeneous Wireless Networks
 - COST Office Asst Prof Mihael Mohorčič
- 12. HiPEAC; European Network of Excellence on High Performance and Embedded

- Architecture and Compilation Ghent University Prof. Roman Trobec
- 13. Cellular and Finite Automata for Structure Recognition
- Slovenian Research Agency Prof. Roman Trobec
- 14. Advanced Technologies for Next Generations of Mobile Broadband Communication Systems
 - Slovenian Research Agency Asst. Prof. Tomaž Javornik
- Optimization of Energy Consumption in Distributed Computing Systems Slovenian Research Agency Prof. Roman Trobec

RESEARCH PROGRAMS

- 1. Telecommunication Systems
- Prof. Gorazd Kandus
- 2. Parallel and Distributed Systems Prof. Roman Trobec

R&D GRANTS AND CONTRACTS

- Learning, Analysis, and Detection of Motion in the Framework of a Hierarchical Compositional Visual Architecture Prof. Roman Trobec
- Model for Domain-Specific Trend Prediction based on Semantic Enrichment of Unstructured Patterns Prof. Roman Trobec
- Advanced Procedures for Interactive Composition of Sensor Networks Asst. Prof. Mihael Mohorčič
- 4. Open Communication Platform for Service Integration: CC OPCOMM Asst. Prof. Mihael Mohorčič
- 5. Cloud Assisted Services: CC CLASS Prof. Roman Trobec
- Efficient Self-Configuration Methods for Wireless Mesh Networks Dr. Carolina Fortuna

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We improved a simulation model for the performance evaluation of network-coding techniques.



NEW CONTRACTS

Technologies for Next-Generation Intelligent Motorhome Adria Mobil, d. o. o., Novo Mesto Asst. Prof. Mihael Mohorčič

VISITORS FROM ABROAD

- 1. Prof. Luiz DaSilva, Department of Electronic and Electrical Engineering, Trinity College Dublin, Dublin, Ireland, 27.-30. 3. 2013
- Camelia Marie Sarosi, Andrei Toma, Ciprian Anton, Technical University of Cluj-Napoca, 2 Faculty for Electronics, Cluj-Napoca, Romania, 1.-15. 9. 2013
- Prof. Veljko Milutinović, Faculty of Electrical Engineering, University of Beograd, 3 Belgrade, Serbia, 8.-12. 7. 2013

- Propagation and Topology Design Evaluation for Wireless Sensor Networks Operating in License Exempt Frequency Bands Cosvlab. d. d. Asst, Prof. Mihael Mohorčič
- Prof. Erich Leitgeb, Institut für Hochfrequenztechnik Graz, University of Technology, 4. Graz, Austria, December 2013
- 5 Prof. Milica Pejanović Djurišić, Ministry of Defense Montenegro, Podgorica, Montenegro, 19.-23. 12. 2013
- Prof. Zoran Veljović, prof. Igor Radušinović, Faculty of Electrical Engineering, University of Montenegro, Podgorica, Montenegro, 19.-23. 12. 2013
- Prof. Karolj Skala, Instituta Ruđer Bošković, Zagreb, Croatia, 16. and 24. 12. 2013

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- Asst. Prof. Mihael Mohorčič, Head 6.
- Asst. Prof. Roman Novak
- 8. Dr. Igor Ozimek
- 9. Dr. Marjan Šterk'
- 10. Asst. Prof. Aleš Švigelj
- 11. Prof. Roman Trobec

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- 13. Dr. Carolina Fortuna
- 14. Dr. Andrej Hrovat 15. Dr. Gregor Kosec

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- 7. Monika Kapus-Kolar, "Error-preserving local transformations on communication protocols", Softw. test. verif. reliab., vol. 23, no. 1, pp. 3-25.2013.
- 8. Monika Kapus-Kolar, "On the use of status messages in checking sequences for the distributed test architecture", Elektrotehniški vestnik, vol. 80, no. 5, pp. 240-244, 2013.
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- 16. Dr. Janez Ivan Pavlič 17. Dr. Andrej Vilhar
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- 18. Kemal Alič, M. Sc.
- 19. Klemen Bregar, B. Sc.
- 20. Urban Kuhar, B. Sc.
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- 22. Dr. Aleksandra Rashkovska
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PUBLISHED CONFERENCE CONTRIBUTION (INVITED

LECTURE)

1. Mihael Mohorčič, "Integration of terrestrial and aiborne wireless networks for emergency situations: the ABSOLUTE project", In: *Telekomunikacijski sistemi u vanrednim situacijama*, IX. međunarodni simpozij iz informacijsko-komunikacijskih tehnologija, INTSIKT 2013, 3-4 juna, 2013, Tuzla, [S. l., s. n.], 2013, 6 pp.

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INDEPENDENT COMPONENT PART OR A CHAPTER IN A

Monograph

- 1. H. P. Hinov, Janez Ivan Pavlič, L. Todorova, Y. G. Marinov, S. Sridevi, M. Slaveikova, A Petrov, P. M. Rafailov, U. Dettlaff-Weglikowska, "Influence of carbon nanotubes and a phospholipid surface layer on the electrooptic behavior of a homeotropic E7", In: *New developments in liquid crystals and applications*, (Materials science and technologies), P. K. Choudhury, ed., New York, Nova Science, 2013, pp. 151-197.
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PATENT APPLICATION

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Patent

- 1. Bojan Likar, Robert Posel, Andreas Kalagasidis, Tomaž Javornik, Gorazd Kandus, Mihael Mohorčič, Aleš Švigelj, Janez Bešter, Andrej Kos, Miha Smolnikar, *Iterative localization techniques*, US8565106 (B2), US Patent Office, 22.10.2013.
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MENTORING

- 1. Carolina Fortuna, *Dynamic composition of communication services:* doctoral dissertation, Ljubljana, 2013 (mentor Mihael Mohorčič; comentor Dunja Mladenić).
- 2. Amir Ligata, *Radio frequency impairments in cooperative broadband wireless communication systems:* doctoral dissertation, Ljubljana, 2013 (mentor Tomaž Javornik; co-mentor Haris Gačanin).
- 3. Aleksandra Rashkovska, *Real-time control of hidden system variables with application in therapeutic knee cooling:* doctoral dissertation, Ljubljana, 2013 (mentor Roman Trobec).
- 4. Ivan Tomašić, *Personalized synthesis of the 12-lead ECG from bipolar leads:* doctoral dissertation, Zagreb, 2013 (mentors Ratko Magjarević, Roman Trobec).

COMPUTER SYSTEMS DEPARTMENT E-7

The Computer Systems department is concerned primarily with the development of advanced computing structures and efficient algorithms for massive-data processing, and systems for effective human-computer interaction. Within this broad area, we are concentrating on self-reparable and self-organizing systems, modeling and optimizing of complex, dynamic and nondeterministic systems. Our research results are implemented within applications for production, transport, energy, environmental sustainability, bioinformatics, health, and medicine. As an integral part of our research activities, members of the department have close contacts and collaborations with scientists world-wide, through academic links and industrial contacts, thus enabling us to keep at the forefront of rapidly developing fields.



In the field of the advanced computer structures we were developing a system for the processing of massive data. Within the application project Processing of massive geometric LIDAR data we developed a hardware accelerator for the compression of LIDAR data. For this purpose, hardware predictors of the point coordinates and Prof. Franc Novak other attributes of LIDAR data were developed. The predictors of the point coordinates consist of two methods: linear prediction using last-coordinate changes, and the search for the closest coordinate change among the most recent

coordinate changes. The applied method is dynamically selected based on the resemblance of the current search result. A pipelined hardware divider, required for linear prediction, was also developed. An adjustable pipeline depth enabled us to select the most suitable divider with respect to the dividers' latency, the usage of the hardware resources, and the clock period. The coordinate prediction and the prediction of other LIDAR data attributes are used in the prediction compression of the LIDAR data. Additionally, a vari-

We developed an e-service and a mobile application "eDietetik" (http://www.edietetik. si/) for patients with special nutritional needs (coeliac disease, diabetes, phenylketonuria and hypertension).

able length encoder was developed, and the arithmetic coder was improved by using the barrel-shifter structure, which resulted in an up to 8-times higher data throughput. Modules were developed in the VHDL language and verified in the Cadence simulation environment. Individual modules were synthesized and tested on the Xilinx XUPV5 prototype board.

We continue the development of self-reparable systems based on FPGA. The SRAM-based field-programmable gate arrays (FPGAs) in mission-critical systems require error mitigation and recovery techniques to protect them from the errors caused by high-energy radiation, also known as single-event upsets (SEUs). We developed a SEU-

recovery mechanism with a smaller hardware overhead than the existing solutions. According to the required levels of reliability, different architectures of the self-recoverable mechanism can be employed. The efficiency of the proposed approach was evaluated with a specially developed fault-emulation environment. In contrast to conventional fault-injection methods based on radiation techniques, the developed fault emulation enables the user to inject faults at selected locations of the configuration memory. Individual parts of the recovery infrastructure can be analyzed using a developed fault-emulation environment. In this way, modifications and possible improvements to the recovery infrastructure can be easily and precisely evaluated. The resulting Figure 1: Open Platform for Clinical Nutrition in the context of various estimated reliability of our error-recovery mechanism is superior to other domestic and international eHealth projects reported solutions.



We developed electronic circuits with advanced functionalities. In collaboration with BSH Hišni aparati, d.o.o., Nazarje, we upgraded the electronic circuits in their household appliances MUM5 and MUMXL. We added electronic circuits to their appliances to implement some additional functionalities, and improve their usability. The developed microcontroller and additional sensors allow the remote monitoring and control of the appliances, while still allowing unchanged functionalities of the original appliances.



Efficient algorithms for computer data-processing

Research in the field of the development of efficient algorithms for computer data processing was focused in the development of computer support for diet planning. We developed an e-service and a mobile application *eDi*-

We introduced a new social network model that takes into consideration the balance theory and stigmergy as a way of interaction between individuals. *etetik* (http://www.edietetik.si/) for patients with special nutritional needs (coeliac disease, diabetes, phenylketonuria and hypertension). The e-service and the application provide, through the food barcode scanning, immediate informing for a user about the composition of the food. In connection with the existing web application *Open Platform for Clinical Nutrition – OPEN* (http://www.opkp.si/). *eDietetik* allows the creation of optimal diet menus with the use of a multi-criteria approach. Within the project *DIETS2* (http://

www.thematicnetworkdietetics.eu/everyone/) we translated the user interface of the OPEN into English and an additional McCance and Widdowson's food composition database was added to the OPEN dataset, to be used by the European Federation of the Association of Dietitians (EFAD).

Within the FP7 European project *EuroFIR NEXUS* (http://www.eurofir.org/) we setup the computer infrastructure (standards, protocols and web services) for the interchange of data of food composition databases between

research institutions and the private sector. OPEN is a part of this infrastructure and allows the interchange of Slovenian food composition data with other research centers in Europe. It is regarded as a national information point. In this context we collaborated with the National Institute for Public Health (NIJZ) when creating the national nutritional profile.

In the FP7 European project *EuroDISH* (http://www.eurodish.eu/) we designed and implemented an algorithm for the semi-automated matching of food consumption and food composition data from various national food databases. By using the algorithm, knowledge from different food data and information sources can be linked, which is particularly important in addressing the issue of food safety. We applied our knowledge from the field of stochastic optimization. The developed algorithm is an important part of the methodology for collecting and analyzing food consumption data, which we develop in collaboration with NIJZ RS. To support this methodology we have upgraded the OPKP platform with a 24h-recall method for collecting and statistically analyzing food-consumption data.

We organized the annual meeting and the conference EuroFIR Nexus *Developments in Food Composition Information Systems supporting ethnic and traditional food in Europe* in Ljubljana. The subject of the conference was the problem of ethical and traditional food from the compositional and informational point of view. We hosted about 100 delegates from 50 European

organizations. Within the conference we also organized the *Workshop of EuroFIR/EuroDISH on Food Matching*, where the delegates from several European research centers discussed the problem of food data matching from the computer-support point of view.

In the field of **s**elf-organizing systems we worked on the parameter-less and self-adaptive control of the optimization algorithms. The effectiveness of the approach, where the user does not need any specific knowledge on control parameter setting, was tested in the context of multi-criteria optimization. The highest usability of the approach is seen in connection with self-organizing emergent systems. For this reason, we study stigmergy, i.e., coordination, where the collective functioning of the system is achieved by indirect interactions between elements of the system. We investigate both sematectonic, as well as sign-based stigmergy. Sematectonic stigmergy denotes communication

via the modification of a physical environment, while sign-based stigmergy denotes communication via a signaling mechanism.

The principle of self-organizing stigmergic systems is used in the implementation of the solutions for optimization procedures within the

ARTEMIS project *Adaptive Cooperative Control in Urban (sub) Systems – ACCUS* (http://www.projectaccus.eu/), where we develop the platform for the integration and coordination of urban systems (transportation, outdoor lighting, energy) to build applications across urban systems, to provide adaptive and cooperative control for urban subsystems, and to optimize the combined performance.

In cooperation with the Department of Intelligent Systems and the Laboratories for Computer Architecture and Languages and Programming Methodologies from the Faculty of Electrical Engineering and Computer Science, University of Maribor, we organized, for the tenth consecutive year, the workshops on *Nature-inspired algorithms* about stochastic optimization techniques.



Figure 2: The MUMXL food mixer with upgraded electronics

We developed a website-usability testing tool.

Human-computer interaction

In the area of human-computer interaction we developed in collaboration with the Faculty of Electrical Engineering and Computer Science, University of Maribor, a website-usability testing tool. The tool can be used for the analysis of visual usability of a website design from the perspective of user cognitive load.

We also participate in an informal community of *Slovenian humancomputer interaction researchers* (http://hci.si/) initiated by the Faculty of Computer and Information Science, University of Ljubljana, XLAB Research, Ljubljana, and the Jožef Stefan Institute. In the frame of the 16th international Information Society – IS 2013 multiconference we organized the conference Human-computer Interaction in Information Society. On this occasion we presented the mobile application *eDietetik* for the presentation of healthrelated information.

In the network modeling studies we discussed three aspects of large graphs. The first aspect represents the network measures and indices that serve as the presentation of the structural graph properties. In this context the focus is given to the Wiener index and the problem of specifying graph families for which the Wiener index equals the Wiener index of its line graph. Additionally, two new centrality indices are introduced, their extreme values are proven and the structures of graphs where these values are achieved are



Figure 3: The social networks modeling

determined. Another aspect relates to the modeling of the social network. It introduced a new social network model, which takes into consideration the balance theory and stigmergy as a way of interaction between individuals. For the evaluation and validation of the model various model characteristics are calculated and analyzed and they are compared to the characteristics of real networks. The last aspect refers to the robustness of the hypercube, which is a frequent topology of parallel networks. We proved that the given upper bound of mutually-independent s-starting Hamiltonian cycles in the hypercube with faulty edges is tight. These three aspects are presented in depth in the PhD thesis *Large graphs in advanced applications*.

In the process of building the methodological framework for analytics technology integration in organizations we addressed the problems and challenges faced by analytics practitioners in the initial stages of technology integration, where its success influences the later phases of integration. The findings may be applied in various analytics domains, i.e., data-mining, forecasting/extrapolation, modeling, simulation, and optimization. To increase the efficiency of the initial analytics we proposed a methodological framework – a system of principles, practices, and procedures. For the data-mining (DM) case, the methodological framework was validated and reported through a series of case studies. Our findings indicate a significant range of considerations and reveal additional issues for applied decision making in the context of DM requirements and process success. Best practices of embryonic DM are expressed by seven success factors and four success measures. Moreover, a process model for carrying out embryonic DM was designed. The methodological framework building and the corresponding research process are presented in the PhD thesis *A Methodological Framework for Integration Of Data Mining in Organizations*.

Some outstanding publications in the past year

- 1. Papa, G.: Parameter-less algorithm for evolutionary-based optimization: for continuous and combinatorial problems, *Computational Optimization and Applications*, 56 (2013) 1, 209–229
- Korošec, P., Šilc, J.: The continuous differential ant-stigmergy algorithm for numerical optimization, *Computational Optimization and Applications*, vol. 56 (2013) 2, 481–502
- Biasizzo, A., Novak, F.: Hardware accelerated compression of LIDAR data using FPGA devices, *Sensors*, 13 (2013) 5, 6405–6422
- Korošec, P., Bole, U., Papa, G.: A multi-objective approach to the application of real-world production scheduling, *Expert Systems with Applications*, 40 (2013) 15, 5839–5853
- Korošec, P., Papa, G.: Metaheuristic approach to transportation scheduling in emergency situations, *Transport*, 28 (2013) 1, 46–59

Organization of conferences, congresses and meetings

- 1. Second Annual Meeting and Conference of EuroFIR Nexus "Developments in Food Composition Information Systems supporting ethnic and traditional food in Europe", Ljubljana, Slovenia, 5.–7. 3. 2013
- 2. Workshop of EuroFIR/EuroDISH "Food Matching", Ljubljana, Slovenia, 8. 3. 2013
- 3. AVN, The 22nd Workshop Nature-Inspired Algorithms, Šmarna Gora, Slovenia, 21. 5. 2013

- 4. HCI - IS, Human-Computer Interaction in Information Society, part of the 16th Information Society Multiconference, Ljubljana, Slovenia, 8. 10. 2013
- 5. AVN, The 23rd Workshop Nature-Inspired Algorithms, Maribor, Slovenia, 16. 12. 2013

INTERNATIONAL PROJECTS

- 7FP EuroFIR-Nexus; The EuroFIR Food Platform: Further Integration, Refinement and 1. Exploitation of for its Long-term
- European Commission Asst. Prof. Barbara Koroušić Seljak
- COST IC1204; Trustworthy Manufacturing and Utilization of Secure Devices 2 COST Office
- Prof. Franc Novak
- HiPEAC; European Network of Excellence on High Performance and Embedded 3. Architecture and Compilation Ghent University
- Prof. Franc Novak 4 EuroFIR AISBL Infrastructure Consultancy EuroFIR AISBL Prof. Peter Korošec
- Upgrade of the Open Platform for Clinical Nutrition to Suit the Needs of the Federation 5. of EU Member National Associations of Dietitians EFAD
- EuroFIR AISBL Asst. Prof. Barbara Koroušić Seljak
- EuroDISH; EuroDISH Determinants-Intake-Status-Health 6 European Commission

Asst. Prof. Barbara Koroušić Seljak

RESEARCH PROGRAM

1. Computer Structures and Systems Prof. Stanislav Kovačič

VISITORS FROM ABROAD

- 1. Prof. Mirjana Gurinović, Prof. Marija Glibetić, Dr. Agnes Kadvan, Jelena Milešević, Ph. D. student, Dr. Snježana Petrović, Slavica Ranković, Ph.D. student, Institute for Medical Research, Belgrade, Serbia, 3.-6. 3. 2013
- Heikki Pakkala, National Institute for Health and Welfare (THL), Finland, 4.-8. 3. 2013 2.
- Tue Christensen, Technical University of Denmark, Denmark, 8. 3. 2013 3.
- Aida Turrini, Istituto Nazionale di Ricerca per gli Alimenti e la Nutrizione (INRAN), 4. Roma, Italy, 8. 3. 2013
- STAFF

Researchers

- Asst. Prof. Anton Biasizzo
- Prof. Peter Korošec
- Asst. Prof. Barbara Koroušić Seljak 3
- 4. Prof. Stanislav Kovačič'
- 5 Prof. Franc Novak, Head
- 6. Asst. Prof. Gregor Papa
- Asst. Prof. Jurij Šilc
- Postdoctoral associates Dr. Drago Torkar 8.

R&D GRANTS AND CONTRACTS

- Processing of Massive Geometric LIDAR Data 1 Prof. Franc Novak
- eDietitian: Mobile Diet Guide 2 Asst. Prof. Barbara Koroušić Seljak
- 3. Adaptive Cooperative Control in Urban (Sub)Systems Asst. Prof. Gregor Papa

NEW CONTRACTS

- Analysis of Possible Upgrades of the A-Portal Web Platform 1. Abak.net, d. o. o.
- Asst. Prof. Gregor Papa 2. Study of the Effects of Upgrading on ISL Online Software Xlab, d. o. o.
 - Asst. Prof. Gregor Papa Energy Efficiency Improvement Study of the Blue Tracker Tracking Device

Ema, d. o. o. Prof. Franc Novak

- Karl Presser, Premotec GmbH, Zurich, Switzerland, 8. 3. 2013 5
- 6. Sandra Crispim, Jan van der Laan, Institut national de la recherche agronomique (INRA), Paris, France, 8. 3. 2013

9. Dr. Vida Vukašinović Postgraduates 10. Lucas Benedičič** 11. Uroš Bole* Technical and administrative staff 12. Jolanda Jakofčič

Note:

* part-time JSI member ** postgraduate financed by industry

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- 1. Anton Biasizzo, "On-line testing and recovery of systems with dynamic partial reconfiguration", *Inf. MIDEM*, vol. 43, no. 4, pp. 259-266, 2013.
- Anton Biasizzo, Franc Novak, "Hardware accelerated compression of LIDAR data using FPGA devices", *Sensors*, vol. 13, no. 5, pp. 6405-6422, 2013.
- Anton Biasizzo, Franc Novak, Peter Korošec, "A multi-alphabet arithmetic coding hardware implementation for small FPGA devices", J. Elektr. Eng., vol. 64, no. 1, pp. 44-49, 2013.
- 4. Mojca Bizjak, Zala Jenko Pražnikar, Barbara Koroušić-Seljak, "Development and validation of an electronic FFQ to assess food intake in the Slovene population", *Public health nutr. (Wallingford. Online)*, ilustr..
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- Uroš Kač, Franc Novak, "Reconfiguration schemes Of SC biquad filters for oscillation based test", *Inf. technol. valdyn.*, vol. 42, no. 1, pp. 38-47, 2013.
- Mojca Korošec, Terezija Golob, Jasna Bertoncelj, Vekoslava Stibilj, Barbara Koroušić-Seljak, "The Slovenian food composition database", In: Food composition and sustainable diets, 9th International Food Data Conference, September 14-17, 2011, Norwich, United Kingdom, *Food Chem.*, vol. 140, no. 3, pp. 495-499, 2013.
- Peter Korošec, Uroš Bole, Gregor Papa, "A multi-objective approach to the application of real-world production scheduling", *Expert syst. appl.*, vol. 40, issue 15, pp. 5839-5853, 2013.
- 9. Peter Korošec, Gregor Papa, "Metaheuristic approach to transportation scheduling in emergency situations", *Transport (Vilnius (Spausd.))*, vol. 28, no. 1, pp. 46-59, 2013.
- Peter Korošec, Jurij Šilc, "The continuous differential ant-stigmergy algorithm for numerical optimization", *Computat. optimiz. appl.*, vol. 56, no. 2, pp. 481-502, 2013.
- 11. Peter Korošec, Marian Vajteršic, Jurij Šilc, Rade Kutil, "Multi-core implementation of the differential ant-stigmergy algorithm for numerical optimization", In: Proceedings of the 14th International Workshop on Nature Inspired Distributed Computing, NIDISC 2011 in conjunction with 25th IEEE/ACM International Parallel and Distributed Processing, IPDPS 2011, May 16-20, 2011 Anchorage, Alaska, USA, J. Supercomput., vol. 63, no. 3, pp. 757-772, 2013.
- 12. Barbara Koroušić-Seljak, Vekoslava Stibilj, Larisa Pograjc, Nataša Fidler Mis, Evgen Benedik, "Food composition databases for effective quality nutritional care", In: Food composition and sustainable diets, 9th International Food Data Conference, September 14-17, 2011, Norwich, United Kingdom, *Food Chem.*, vol. 140, no. 3, pp. 495-499, 2013.
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- 16. Peter Novak, Franc Novak, Barbara Koroušić-Seljak, "Enhancement of web application design of the open platform for clinical nutrition", In: Human factors in computing and informatics: proceedings, First International Conference, SouthCHI 2013, Maribor, Slovenia, July 1-3, 2013, Lect. Notes Comput. Sci., vol. 7946, pp. 791-802, 2013.
- 17. Gregor Papa, "Parameter-less algorithm for evolutionary-based optimization: for continuous and combinatorial problems", *Computat. optimiz. appl.*, vol. 56, issue 1, pp. 209-229, 2013.

- 18. Janez Perš, Matej Kristan, Rok Mandeljc, Stanislav Kovačič, Aleš Leonardis, "Hierarhična kompozicionalna arhitektura za detekcijo in razpoznavanje aktivnosti", *Elektrotehniški vestnik*, vol. 80, no. 5, pp. 258-265, 2013.
- Mitja Placer, Stanislav Kovačič, "Enhancing indoor inertial pedestrian navigation using a shoe-worn marker", *Sensors*, vol. 13, no. 8, pp. 9836-9859, Aug. 2013.
- 20. Nada Rotovnik-Kozjek, Živa Mrevlje, Barbara Koroušić-Seljak, Katja Kogovšek, Branko Zakotnik, Iztok Takač, Matjaž Horvat, Tadej Dovšak, Vojislav Didanovič, Andrej Kansky, Jožica Červek, Vaneja Velenik, Franc Anderluh, Milena Kerin-Povšič, Matjaž Sever, Primož Strojan, Borut Štabuc, Mojca Unk, Jernej Benedik, Erik Brecelj, Tadeja Pintar, Lidija Kompan, Marko Novak, Laura Petrica, Denis Mlakar-Mastnak, Brigita Avramović Brumen, Eva Peklaj, Rajmonda Jankovič, Urška Jelenko, Edita Rotner, Sanja Đukić, Petra Tavčar, "Kaheksija pri bolnikih z rakom", Zdrav Vestn (Tisk. izd.), vol. 82, no. 3, pp. 133-141, mar. 2013.
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PUBLISHED CONFERENCE CONTRIBUTION

- Anton Biasizzo, "On-line testing and recovery of systems with dynamic partial reconfiguration", In: *Proceedings*, 49th International Conference on Microelectronics, Devices and Materials & theWorkshop on Digital Electronic Systems, September 25 - September 27, 2013, Kranjska Gora, Slovenia, Andrej Žemva, ed., Polona Šorli, ed., Iztok Šorli, ed., Ljubljana, MIDEM - Society for Microelectronics, Electronic Components and Materials, 2013, pp. 13-19.
- 2. Peter Korošec, Jurij Šilc, "The continuous differential ant-stigmergy algorithm applied on real-parameter single objective optimization problems", In: *IEEE Congress on Evolutionary Computation*, [2013 IEEE CEC], June 20-23, 2013, Cancun, Mexico, [S. l.], IEEE, cop. 2013, pp. 1658-1663.
- 3. Barbara Koroušić-Seljak, "How to provide health-related information by mobile computing?", In: *Zbornik 16. mednarodne multikonference Informacijska družba - IS 2013, 7.-11. oktober 2013* [Ljubljana, *Slovenija*]: *zvezek A: volume A*, Matjaž Gams, ed., et al, Ljubljana, Institut Jožef Stefan, 2013, pp. 225-228.
- 4. Franc Novak, Denis Špelič, Borut Žalik, "A website usability testing tool", In: Zbornik 16. mednarodne multikonference Informacijska družba - IS 2013, 7.-11. oktober 2013 [Ljubljana, Slovenija]: zvezek A: volume A, Matjaž Gams, ed., et al, Ljubljana, Institut Jožef Stefan, 2013, pp. 217-220.
- Gregor Papa, Jurij Šilc, "The parameter-less evolutionary search for real-parameter single objective optimization", In: *IEEE Congress on Evolutionary Computation*, [2013 IEEE CEC], June 20-23, 2013, Cancun, Mexico, [S. l.], IEEE, cop. 2013, pp. 1131-1137.
- 6. Miha Ristič, Franc Novak, "Towards improved emergency call service: a usability test case study", In: *Zbornik 16. mednarodne multikonference Informacijska družba IS 2013, 7.-11. oktober 2013 [Ljubljana, Slovenija]: zvezek A: volume A*, Matjaž Gams, ed., et al, Ljubljana, Institut Jožef Stefan, 2013, pp. 229-232.

MENTORING

- 1. Uroš Bole, *A methodological framework for integration of data mining in organizations:* doctoral dissertation, Ljubljana, 2013 (mentor Gregor Papa).
- Vida Vukašinović, Large graphs in advanced applications: doctoral dissertation, Ljubljana, 2013 (mentor Jurij Šilc; co-mentor Riste Škrekovski).

DEPARTMENT OF KNOWLEDGE **TECHNOLOGIES** E-8

The Department of Knowledge Technologies performs research in advanced information technologies aimed at acquiring, storing and managing knowledge to be used in the development of knowledge-based applications. Established areas include intelligent data analysis (machine learning, data mining, and knowledge discovery in databases), semantic data mining and the semantic web, language technologies and computational linguistics, decision support and knowledge management. Apart from research in knowledge technologies, we are also developing applications in environmental sciences and ecology, medicine and health care, biomedicine and bioinformatics, economy and marketing.

In 2013 we were involved in six national and eleven FP7 projects, two COST actions, one network financed by the European Science Foundation, one infrastructure project and two industry projects.

In the area of intelligent data analysis and data mining we have developed several new methods and used them in a number of application domains. In collaboration with the University of Helsinki we have developed a new Head: method for contrasting subgroup discovery and successfully applied it to the analysis of differential gene expres- Prof. Nada Lavrač sion of virus-infected potato plants, aimed at improved understanding of the plants' response to virus attack. We developed a methodology for analyzing text-enriched heterogeneous information networks, which was successfully applied in the analysis of video lectures on the VideoLectures.net portal. The developed NoiseRank methodology for ensemble-based noise and outlier detection was applied to a medical problem domain and the detection of atypical

newspaper articles. A new platform ViperCharts enables the visualization of noise-detection performance results as well as a visual evaluation of the quality of information-extraction algorithms. We developed a new propositionalization method, named wordification, for transforming relational data into bag-of-words vectors: the method, which was successfully applied to data in the IMDB film database, is made available within the ClowdFlows web platform, which supports data analysis in the cloud. The banded matrices

methodology has been applied in a new task of cross-domain narrative ideation. We developed a new sentiment analysis methodology, which was successfully applied in a sentiment analysis of financial tweets. We improved the HCI interface of the CrossBee bisociation knowledge discovery system, which can be used for the analysis of scientific articles with the aim of discovering new links between different domains.

We continued our successful collaboration in the FP7 FET project MUSE (Machine Understanding for interactive StorytElling) in the area of the computer understanding of natural language, the goal of which is to convert text

into its 3D animation. In October 2013 we started a collaboration in two new FP7 computational creativity projects, ConCreTe (Concept Creation Technologies) and WHIM (The What-If Machine), while continuing the collaboration in the FP7 coordination action PROSECCO, whose goal is the promotion of activities in the area of computational creativity.

We have developed new methods for learning decision trees and ensembles for structured output prediction (multi-target classification and regression and (hierarchical) multi-label classification), some of which can also take into account the spatial or network location of specific examples. New methods were used for searching and labeling images, modeling of dynamic systems and for different problems in the area of environmental sciences, such as the habitat modeling of various organisms and the modeling of gene flow between conventional and genetically modified crops. In the area of life sciences we have used the newly developed methods for identifying relations

between health state and gut microbiota composition, and for gene-function prediction, where we have produced more than 400,000 reliable function predictions for genes from about a thousand bacterial genomes (the predictions are available on server http://gorbi.irb.hr/), and we have contributed to a comprehensive overview study of computational methods for gene-function prediction.

and development.

Nada Lavrač received the Zois Recognition Award for her work in intelligent data analysis. The awards are given annually to Slovene scientists for important contributions to science, research

the reputation of financial institutions, the detection of financial manipulations, assistance in stock trading, and for monitoring of events connected to the current financial crisis.

Figure 1: In the FP7 project FIRST we developed systems for evaluating





We have further developed methods for learning models of dynamical systems from data and domain background knowledge and considered different methods and criteria for parameter optimization as well as ensembles of such models. This research was part of the F7P project SUMO (Supermodeling by combining imperfect models). These methods were also used for the modeling of aquatic ecosystems and the process of endocytosis, which is a key part of the immune system. In the FP7 project REWIRE (Rehabilitative Wayout In Responsive home Environments), which aims at the development of a rehabilitation system for post-stroke patients, we have applied methods for machine learning to analyze patient data together with data collected from wearable sensors. The aim was to monitor patient rehabilitation and to design an adaptive rehabilitation plan.

In the area of text and web mining and heterogeneous information network analysis we continued our research in the framework of four FP7 projects. FIRST (Large scale information extraction and integration infrastructure for supporting financial decision making) was successfully concluded in October 2013 with an excellent final evaluation. FOC (Forecasting Financial Crises) is about to be concluded in February 2014. We started work on two new

Marko Bohanec and co-authors received the Outstanding Paper Award at the 26th Bled eConference for their contribution "Hot stock or not? A qualitative multi-attribute model to detect financial market manipulation". projects, SIMPOL (Financial Systems Simulation and Policy Modelling) and MULTIPLEX (Foundational Research on MULTIlevel comPLEX networks and systems). We focused on analyzing large amounts of dynamic and heterogeneous sources of financial information and developed online datamining tools for the near-real-time processing of vast amounts of constantly evolving data (financial news, blogs and tweets). We permanently monitored 200 financial websites, capturing about 40,000 documents per day. In 2013

we focused on data analysis and end-user solutions, such as a sentiment analysis on financial products, estimating the reputation of financial institutions, and on-online fraud detection. In FOC we extracted indicators based on the sentiment analysis of large streams of textual data, with the goal of forecasting financial crises. The SIMPOL project is intended as a support for decision makers and regulators in policy modeling and impact analysis, with the emphasis on climate finance and regulations. The main goal of MULTIPLEX is oriented towards the use of the mathematical framework of Complex Networks and Algorithmics to establish a theoretical basis for the understanding, prediction and, possibly, the control of Complex Systems.

During the parliamentary elections in Bulgaria, in May 2013, we launched a public-sentiment monitoring solution in collaboration with Gama System. We developed a sentiment analysis system that collected and analyzed tweets about the major political parties. The sentiment charts were shown in real time on a web portal, before and during the elections. It turns out that the cumulative sentiment (the difference between the number of positive and negative tweets) very accurately reflects the actual elections results. The parties that won the highest number of



Figure 2: We developed a new method for the computational annotation of gene functions, which is based on the principles of homology and phylogenetic profiles and was published in the PLOS Computational Biology journal.

parliamentary seats had the highest cumulative sentiment, albeit with the inverted sign (i.e., a party with the highest number of negative tweets won the highest number of seats in the newly elected parliament).

In the area of language technologies we concluded with the compilation of language resources of historical Slovene, which contain a digital library of older Slovene literature with facsimiles and hand-corrected and marked-up transcriptions (over 600 books, 45,000 pages), a hand-annotated corpus with modernized word-forms and other linguistic mark-up (300,000 tokens, 1,100 pages) and a lexicon giving glosses for archaic words (20,000 entries, 70,000 word-forms). All the resources are encoded using the TEI P5 Guidelines and available on the Web for reading and searching, as well as for download in the source XML format under the CC-BY license. These resources are already used for teaching the history of Slovene language and literature at several university departments and secondary schools. On the basis of the produced resources we developed a method for modernizing old words, which uses statistical machine translation, although not on words but characters. In the context of our research on the normalization of non-standard language we also studied the behavior of Slovene clitics in older texts and made a preliminary analysis of the differences between the language of tweets and standard Slovene.

After the completion of the project "Slovene translation studies – resources and research" we summarized our work on the linguistic annotation of parallel bi-lingual corpora in the textbook published in the scope of the project. The project "Communication in Slovene", which compiled a new generation of Slovene reference corpora, also ended in 2013. We mounted the corpora of the project, as well as all the others that our department helped to compile, under the high-performance noSketchEngine concordancer and the CUWI concordancer, developed by us. Linguists from Slovenia and abroad are now able to use advanced analytical techniques on over 30 different corpora, spanning reference corpora of contemporary and historical Slovene, specialized corpora from various domains, multilingual parallel corpora, to several large foreign language corpora.

In the project "Leading Slovene Humanists from the 16th to the mid-19th Century" we continued with our work on IT support, developing a tool to produce digital text-critical editions with Word files as the input and TEI P5 documents as the output. In the new project "Slovenian Literature in Unknown Early Modern Manuscripts: Information Technology Aided Analyses and Scholarly Editions" we started work on the automatic modernization of the diplomatic and critical transcriptions of manuscripts. We also cooperated with the Slovenian Academy of Sciences and Arts on producing their Web-based Slovene Biographical Lexicon.

We continued our work in the context of the ESF network NetWordS (European Network on Word Structure) and the COST action MUMIA (Multilingual and Multifaceted Interactive Information Access) and joined the new

COST action PARSEME (Parsing and Multi-word Expressions). We collaborated in the work of the Slovene Institute of Standardization as the Slovene representatives in ISO/TC37/SC4 (Terminology and Other Language and Content Resources / Language Resources Management) by reviewing, translating and approving Slovene standards from this field. We collaborated with the Slovenian Ministry of Culture in preparing the Action Plan for the National Program for Language Policy 2014-2018 and in taking the steps necessary for Slovenia to join the research infrastructure CLAPIN (Common Language Policy

We were the main technological partner in the FP7 project FIRST, which received an excellent score in its final evaluation. For our three-year work on the analysis of financial news, blogs and tweets we received €750,000.

Slovenia to join the research infrastructure CLARIN (Common Language Resources and Technology Infrastructure). In the area of decision support our long-term goal is to develop methods and techniques for decision modeling, support them with software and integrate them with data-mining systems. In 2013 we achieved the most important results in the FP7 project FIRST, in which we developed decision-support models and systems in banking and financial management. One of the solutions is aimed at the detection of fraudulent behavior (the so-called "Pump and Dump" scenarios) in financial transactions. The solution was presented in an awarded conference paper and is implemented in an information system of the project partner bNext from Germany. Another solution is aimed

at bank-reputation risk assessment and is used by the project partner Banca Monte dei Paschi di Siena in Italy. Important theoretical and methodological advancements were achieved by the development of new methods for the ranking of alternatives in qualitative multi-attribute models, which are based on copulas; they improve the sensitivity of decision models and alleviate some drawbacks of existing methods. We developed a database of qualitative decision models, which currently contains over 500 models and will serve as an important resource for forthcoming research. We extended and updated our decision-support software: our flagship decision-modeling program DEXi and open-source library JDEXi were upgraded to a new development platform and extended with a number of functions. In addition to the already-mentioned areas of banking and finance, we applied these methods for the evaluation of water sources and cropping systems, and in the area of providing sustainable energy sources in Slovenia until 2030.

We participated in the project EVADIFF (Evaluation et de développement et modèles outils d'aide à la décision utilisés pour la Prevention des pollutions diffuses par les produits phytopharmaceutiques), commissioned by ARVALIS Institut du Vegetal, France, where we are developing a decision-support system for the selection of mitigation measures for the protection of surface waters from pollution by phytopharmaceuticals. We have implemented the first validated results as an internet application for the internal use of the ARVALIS institute.



Figure 3: The system for home rehabilitation developed within the FP7 project REWIRE.

Some outstanding publications in the past year

- Bohanec, M., Bertheau, Y., Brera, C., Gruden, K., Holst-Jensen, A., Kok, E.J., Lécroart, B., Messéan, A., Miraglia, M., Onori, R., Prins, T. W., Soler, L.-G., Žnidaršič, M.: The Co-Extra decision support system: A model-based integration of project results. Genetically modified and non-genetically modified food supply chains: Co-existence and traceability (ed. Bertheau, Y.), Wiley-Blackwell, 2013, 461–489
- Erjavec, T., Jelovšek, A.: A corpus-based diachronic analysis of Slovene clitics. V: Bennett, P. (ed.). New methods in historical corpora, (Korpuslinguistik und interdisziplinäre Perspektiven auf Sprache = Corpuslinguistics and interdisciplinary perspectives on language). Tübingen: Narr Verlag, 2013, 117–126

- Grčar, M., Trdin, N., Lavrač, N.: A methodology for mining document-enriched heterogeneous information 3. networks. The Computer journal, 2013, vol. 56, no. 3, 321-335
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Awards and appointments

- Marko Bohanec: Best paper reward on International Conference 26th Bled eConference eInnovation: Chal-1. lenges and Impacts for Individuals, Organizations and Society
- Sašo Džeroski, Nikola Simidjievski, Ljupčo Todorovski: Best ICT paper on 5th Jožef Stefan International Post-2. graduate School Students Conference
- 3. Nada Lavrač: Zois Recognition Award for her work in intelligent data analysis, Applicant: Committee of the Republic of Slovenia Zois Award
- Vid Podpečan: The outstanding scientific achievement: Environment Orange4WS for service-oriented data min-4. ing, Applicant: Public Research Agency of the Republic of Slovenia (SRA), the Scientific Council for Engineering
- 5. Nejc Trdin: Award to Organising Committee for creativity, ideas, help and support in organizing 5th Jožef Stefan International Postgraduate School Students Conference, Applicant: Dean and President of Jožef Stefan International Postgraduate School

Organization of conferences, congresses and meetings

- Project meeting of European project SUMO, Ljubljana, Slovenia, 6.-7. 5. 2013 1.
- Project meeting of European project FIRST, Dubrovnik, Croatia, 12.-14. 6. 2013 2.
- Symposium machine learning and computational creativity, Ljubliana, Slovenia, 4.7. 2013 3.
- 4. Project meeting of European project MUSE, Ljubljana, Slovenia, 30. 9.-2. 10. 2013

INTERNATIONAL PROJECTS

- EVADIFF; Evaluation of Existing Models and Development of New Decision-making Tools to prevent Diffuse Pollution caused by Plant Protection Products Arvalis - Înstitut du Végétal Prof. Marko Debeljak
- 2. 7FP - FIRST; Large Scale Information Extraction and Integration Infrastructure for Supporting Financial Decision Making
- European Commission Prof. Nada Lavrač
- 7FP SUMO; Supermodeling by Combining Imperfect Models 3 European Commission
- Prof. Sašo Džeroski 4.
- 7FP FOC-II; Forecasting Financial Crises European Commission Dr. Igor Mozetič
- 7FP REWIRE; Rehabilitative Wayout In Responsive Home Environments European Commission
- Prof. Sašo Džeroski 6. 7FP - MUSE; Machine Understanding for Interactive Storytelling European Commission
- Prof. Nada Lavrač
- 7FP PROSECCO; Promoting the Scientific Exploration of Computational Creativity

European Commission	
Prof. Nada Lavrač	

- 7FP ConCreTe; Concept Creation Technology 8. European Commission Prof Nada Lavrač
- 9 7FP - WHIM: The What-If Machine European Commission
- Prof. Nada Lavrač
- 10 7FP - DECATHLON; Development of Cost Efficient Advanced DNA-Based Methods for Specific Traceability Issues and High Level On-site Applications European Commission
- Prof. Marko Bohanec
- 11 7FP - SIMPOL; Financial Systems Simulation and Policy Modelling European Commission Dr. Igor Mozetič
- 7FP MULTIPLEX; Foundational Research on Multilevel Complex Networks and Systems 12. European Commission Dr. Igor Mozetič
- COST IC1002; MUMIA; Multilingual and Multifaceted Interactive Information Access COST Office
- Dr. Igor Mozetič The European Network on Word Structure European Science Foundation Asst. Prof. Tomaž Erjavec
- 15. PARSEME: PARSing and Multi-Word Expressions; Towards Linguistic Precision and Computational Efficiency in Natural Language Processing COST Office
 - Asst. Prof. Tomaž Erjavec
- Structured Annotation, Storage and Retrieval of Images and Videos Slovenian Research Agency Prof. Sašo Džeroski

RESEARCH PROGRAM

 Knowledge Technologies Prof. Nada Lavrač

R&D GRANTS AND CONTRACTS

- Growth and Defense Trade-offs in Multitrophic Interaction between Potato and Its Two Major Pests Prof. Nada Lavrač
- The Leading Humanists in the Slovenian Territory between the 16th and mid-19th Centuries and Their Social and Cultural Environment Asst. Prof. Tomaž Eriavec

VISITORS FROM ABROAD

- Bogdan Okreša Djurić, University of Varažidn, Faculty of Organization and Informatics, Varaždin, 24. 1.–29. 3. 2013
- 2. Sebastian Dumančić, Zagreb, Croatia, 4.-8. 3. 2013 and 1.-26. 7. 2013
- 3. Dr. Aalar Kuusik, Tallinn University of Technology, Talin, Estonia, 7. 3. 2013
- Prof. Filip Železny, Department of Cybernetics, Faculty of Electrical Engineering, Czech Technical University in Prague, Prague, Czech Republic, 24.–26. 3. 2013
- Prof. Hannu Toivonen, University of Helsinki, Helsinki, Finland, 2.-5. 7. 2013
 Prof. Juergen Kurths, Potsdam Institute for Climate Impact Research, Potsdam.
- Germany, 8. 5. 2013
 Prof. June 6 Annual Magnetic International International Action of Changes and Action Proceedings. J. Control 1997; 1997.
- Prof. Ljupčo Kocarev, Macedonian Academy of Sciences and Arts, Skopje, Macedonia, 8. 5. 2013
- Dr. Wim Wiegerinck, Radboud University Nijmegen, Nijmegen, The Netherlands, 8. 5. 2013
- Dr. David Cornforth, School of Design, Communication and IT, University of Newcastle, Sydney, Australia, 8.–15. 6. 2013
- Dr. Herbert Jelinek, Khalifa University of Science, Technology & Research (KUSTAR), Abu Dhabi, UAE, 8.–15. 6. 2013
- 11. Prof. Don Hodges, University of Tennessee, Institute of Agriculture, Knoxville, USA, 20.–24. 5. 2013
- 12. Dr. Pierre Geurts, University of Liège, Department of Electrical Engineering and Computer Science, Institut Montefiore, Liege, Belgium, 4.–7.6. 2013
- 13. Prof. Jochen Rink, Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany, 3.–5. 6. 2013

STAFF

Researchers

- 1. Prof. Marko Bohanec
- 2. Prof. Bojan Cestnik*
- 3. Prof. Marko Debeljak
- 4. Prof. Sašo Džeroski
- 5. Asst. Prof. Tomaž Erjavec
- 6. Prof. Nada Lavrač, Head
- 7. Prof. Tanja Urbančič*
- Postdoctoral associates
- Dr. Darko Cherepnalkoski
 Dr. Matiaž Iuršič
- 9. Dr. Matjaž Juršič
- 10. Dr. Dragi Kocev
- Dr. Petra Kralj Novak
 Dr. Panče Panov
- 13. Dr. Vid Podpečan
- 14. Dr. Ivica Slavkov
- 15. Dr. Aneta Trajanov
- 16. Asst. Prof. Bernard Ženko
- 17. Asst. Prof. Martin Žnidaršič
- Postgraduates
- 18. Miha Grčar, B. Sc.

- Slovenian Literature in Unknown Early Modern Manuscripts: Information-Technology Aided Analyses and Scholarly Editions Asst. Prof. Tomaž Eriavec
- Development and Applications of New Semantic Data Mining Methods in Life Sciences Prof. Nada Lavrač
- 5. Ecological Restoration of Natural Disturbances in Forests Prof. Marko Debeljak
- 6. Workflows in the Cloud
- Dr. Darko Cherepnalkoski
- 7. Sentiment analysis
- Dr. Matjaž Juršič 8. Google Digital Humanities Award for "Developing Language Models for Historical Slovenian"
- Asst. Prof. Tomaž Erjavec 9. DS/ALT 2014 - The 17th International Conference on Discovery Science and The 25th International Conference on Algorithmic Learning Theory Prof. Sašo Džeroski

NEW CONTRACT

- Shallow Semantic Analyses for Selected European Languages Gama System, d. o. o. Dr. Igor Mozetič
- Shang Yun Liu, Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany, 3.-7. 6. 2013
- 5. Dr. Richard Wheeler, University of Edinburgh, Edinburgh, Scotland, 3.-7. 7. 2013
- Dr. Benoit Real, Dr. Jonathan Marks-Perreau, ARVALIS Institut du végétal, Paris, France, 28.–30. 8. 2013
- Prem Raj Adhikari, Department of Information and Computer Science, Aalto University School of Science, Espoo, Finland, 14.–20. 9. 2013
- Prof. Marie-Francine Moens, Department of Computer Science Katholieke Universiteit Leuven, Leuven, Belgium, 30. 9.–2. 10. 2013
- Prof. Marc Cavazza, Teesside University, Middlesbrough, Great Britain, 30. 9.-2. 10. 2013
- 20. Dr. Tomislav Šmuc, Institut Rudjer Bošković, Zagreb, Croatia, 3.-4. 10. 2013
- 21. Matija Piškorec, Institut Rudjer Bošković, Zagreb, Croatia, 3.-4. 10. 2013
- 22. Vinko Zlatić, Institut Rudjer Bošković, Zagreb, Croatia, 3.-4. 10. 2013
- Dr. Dragan Gamberger, Institut Rudjer Bošković, Zagreb, Croatia, 3.-4. 10. 2014
 Katarina Trojachanec, Faculty of Computer Science and engineering, University Ss.
- Cyril and Methodius, Skopje, Macedonia, 29. 10.–28. 11. 2013 25. Ivan Kitanovski, Faculty of Computer Science and engineering, University Ss. Cyril and
- Methodius, Skopje, Macedonia, 22. 11.–23. 12. 2013
 26. Dr. Gjorgji Madjarov Faculty of Electrical Engineering and Information Technologies, University Ss. Cyril and Methodius, Skopje, Macedonia, 14.–22. 12. 2013
- 19. Dr. Elena Ikonomovska, left 01.02.13
- 20. Jan Kralj, B. Sc
- Janez Kranjc, B. Sc.
 Jurica Levatić
- 23. Dr. Biljana Mileva Boshkoska
- 24. Aljaž Osojnik
- 25. Matic Perovšek, B. Sc.
- 26. Senja Pollak, B. Sc.
- 27. Nikola Simidjievski, B. Sc.
- 28. Borut Sluban, B. Sc.
- 29. Nejc Trdin, B. Sc.
- 30. Anže Vavpetič, B. Sc.
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- Technical and administrative staff
- 32. Tina Anžič, B. Sc.
- 33. Milica Bauer, B. Sc.
- Note: * part-time JSI member

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- 14. Nada Lavrač, Petra Kralj Novak, "Relational and semantic data mining for biomedical research", *Informatica (Ljublj.)*, vol. 37, no. 1, pp. 35-39, 2013.
- 15. Jurica Levatić, Jasna Ćurak, Marijeta Kralj, Tomislav Šmuc, Maja Osmak, Fran Supek, "Accurate models for P-gp drug recognition induced from a cancer cell line cytotoxicity screen", *J. med. chem.*, vol. 56, no. 14, pp. 5691-5708, 2013.
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- 31. Jovan Tanevski, Ljupčo Todorovski, Yannis Kalaidzidis, Sašo Džeroski, "Inductive process modeling of Rab5-Rab7 conversion in endocytosis", In: Discovery science: 16th International Conference, DS 2013, Singapore, October 6-9, 2013, proceedings, *Lect. Notes Comput. Sci.*, vol. 8140, pp. 265-280, 2013.
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PUBLISHED CONFERENCE CONTRIBUTION (INVITED

LECTURE)

 Tomaž Erjavec, "Slovene corpora for corpus linguistics and language technologies", In: *Natural language processing, corpus linguistics, elearning: proceedings*, Seventh International Conference, SLOVKO 2013, November 13-15, 2013, Bratislava, Slovakia, Katarína Gajdošová, ed., Adriána Žáková, ed., [S. l.], RAM-Verlag, 2013, pp. 51-61.

PUBLISHED CONFERENCE CONTRIBUTION

1. Irina Alić, Michael Siering, Marko Bohanec, "Hot stock or not?, A qualitative multi-attribute model to detect financial market

manipulation", In: *elnnovation: challenges and impacts for individuals, organizations and society: conference proceedings,* 26th Bled eConference, June 9-13, 2013, Bled, Slovenia, Dianne L. Wigand, ed., et al, Kranj, Moderna organizacija, 2013, pp. 64-77.

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- Marko Debeljak, Vladimir Kuzmanovski, Florence Leprince, Benot Réal, Sašo Džeroski, Aneta Trajanov, "Prediction of drainage periods and drainage outflow", In: YORK 2013: pesticide behaviour in soils, water and air: 2-4 September 20013, York, UK, York, University of York, 2013, 3 pp.
- 4. Tomaž Erjavec, Alenka Jelovšek, "A corpus-based diachronic analysis of Slovene clitics", V: New methods in historical corpora: [selected papers presented at Conference on New Methods in Historical Corpora, 29th to 30th April 2011, Manchester, UKJ, (Korpuslinguistik und interdisziplinäre Perspektiven auf Sprache = Corpuslinguistics and interdisciplinary perspectives on language, Bd. 3), Paul Bennett, ur., Tübingen, Narr Verlag, 2013, str. 117-126.
- 5. Tina Jaklič, Luka Juvančič, Marko Debeljak, "Incorporation of emergy analysis into decision-making at the farm level: a conceptual model and its implications for agri-environmental policy design", In: *Emergy* synthesis 7: theory and applications of the emergy methodology, Seventh Biennial Emergy Conference, Gainesville, Florida, January, 12-14, 2012, Mark Theodore Brown, ed., Gainesville, The Center for Environmental Policy, University of Florida, 2013, pp. 283-292.
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- 9. Vladimir Kuzmanovski, Marko Debeljak, Sašo Džeroski, "Time-window selection for optimal generalization with noise variance reduction in ecological data", In: *Zbornik*, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 148-157.
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- 11. Jurica Levatić, Dragi Kocev, Sašo Džeroski, "The use of the label hierarchy in HMC improvesperformance: a case study in predictingcommunity structure in ecology", In: *New frontiers in mining complex patterns*, ECML PKDD European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases, September 23-27, 2013, Prague, Czech Republic, [S. I., s. n.], 2013, pp. 189-201.
- 12. Jurica Levatić, Živa Ramšak, Tjaša Stare, Dragi Kocev, Kristina Gruden, Sašo Džeroski, "Gene function prediction for Solanum tuberosum from time-series gene expression data", In: *Zbornik*, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 158-167.
- 13. Fabien Massé, Anisoara Paraschiv-Ionescu, Bernard Ženko, Sašo Džeroski, Kamiar Aminian, "Lifestyle evaluation using wearable technologies: opportunities for stroke patients", In: *Converging clinical and engineering research on neurorehabilitation*, (Biosystems & Biorobotics), International Conference on Neurorehabilitation, ICNR 2012, Toledo, Spain, November 14-16, 2012, José L. Pons, ed., Diego Torricelli, ed., Marta Pajaro, ed., Heidelberg [etc.], Springer, cop. 2013, vol. 1, pp. 941-945.
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Conference on Bioinformatics and Biomedical Engineering, March 18-20, 2013, Granada, [Sl. l., s. n.], 2013, pp. 1-9.

- 15. Patrik Mouron, Marko Bohanec, "A multi-attribute decision method for assessing the overall sustainability of crop protection strategies: a case study based on apple production in Europe", V: Methods and procedures for building sustainable farming systems: [presented at 9th European IFSA Symposium in Vienna, July 2010], Oxford, Elsevier, 2013, str. 123-140.
- 16. Vid Podpečan, Dragana Miljković, Marko Petek, Tjaša Stare, Kristina Gruden, Igor Mozetič, Nada Lavrač, "Integrating semantic transcriptomic data analysis andknowledge extraction from biological literature", In: *Proceedings*, 2013 IEEE International Conference on Bioinformatics and Biomedicine Workshops BIBM 2013, Shanghai, China, December 18-21, 2013, Danvers, Institute of Electrical and Electronics Engineers, 2013, pp. 477-480.
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- Ivica Slavkov, Jana Karcheska, Dragi Kocev, Slobodan Kalajdziski, Sašo Džeroski, "Extending reliefF for hierarchical multi-label classification", In: *New frontiers in mining complex patterns*, ECML PKDD European Conference on Machine Learning and Principles and Practice of Knowledge Discovery in Databases, September 23-27, 2013, Prague, Czech Republic, [S. l., s. n.], 2013, pp. 156-167.
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- 21. Mateja Škerjanec, Darko Čerepnalkoski, Sašo Džeroski, Boris Kompare, Nataša Atanasova, "Modelling dynamic systems using a hybrid approach", In: *Machine Learning in Water Systems: [Proceedings of the AISB Convention 2013, Exeter, UK, 3.-5. April 2013*, Dragan Savić, ed., Exeter, University of Exeter, 2013, pp. 35-38.
- 22. Jovan Tanevski, Ljupčo Todorovski, Sašo Džeroski, "Automated modeling of Rab5Rab7 conversion in endocytosis", In: *Zbornik*, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 209-218.
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- 24. Anže Vavpetič, Petra Kralj Novak, Nada Lavrač, "Analysing financial vocabulary using a new semantic subgroup discovery system Hedwig", In: *Zbornik*, 5. študentska konferenca Mednarodne podiplomske šole Jožefa Stefana = 5th Jožef Stefan International Postgraduate School Students Conference, 23. maj 2013, Ljubljana, Slovenija, Nejc Trdin, ed., et al, Ljubljana, Mednarodna podiplomska šola Jožefa Stefana, 2013, pp. 219-229.
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MONOGRAPH

- Marko Bohanec *et al.* (13 authors), "The Co-Extra decision support system: a model-based integration of project results", In: *Genetically* modified and non-genetically modified food supply chains: co-existence and traceability, Yves Bertheau, ed., Chichester, Blackwell, cop. 2013, pp. 459-489.
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- Tomaž Erjavec, Darja Fišer, "Jezik slovenskih tvitov: korpusna raziskava", In: Družbena funkcijskost jezika: (vidiki, merila, opredelitve), (Obdobja, 32), Andreja Žele, ed., 1. natis, Ljubljana, Znanstvena založba Filozofske fakultete, 2013, pp. 109-116.
- 4. Arne Holst-Jensen *et al.* (28 authors), "Towards detection of unknown GMOS", In: *Genetically modified and non-genetically modified food supply chains: co-existence and traceability*, Yves Bertheau, ed., Chichester, Blackwell, cop. 2013, pp. 367-382.
- 5. Roberta Onori *et al.* (29 authors), "GMO sampling strategies in food and feed chains", In: *Genetically modified and non-genetically modified food supply chains: co-existence and traceability*, Yves Bertheau, ed., Chichester, Blackwell, cop. 2013, pp. 243-272.

MENTORING

- 1. Biljana Mileva Boshkoska, *From qualitative to quantitative evaluation methods in multi-criteria decision models:* doctoral dissertation, Ljubljana, 2013 (mentor Marko Bohanec).
- 2. Darko Čerepnalkoski, *Process-based models of dynamical systems: representation and induction:* doctoral dissertation, Ljubljana, 2013 (mentor Sašo Džeroski; co-mentor Ljupčo Todorovski).
- Matjaž Juršič, Text mining for cross-domain knowledge discovery: doctoral dissertation, Ljubljana, 2013 (mentor Nada Lavrač; comentor Bojan Cestnik).
- 4. Dragana Miljković, *Semi-automated knowledge elicitation for modelling plant defence response:* doctoral dissertation, Ljubljana, 2013 (mentor Nada Lavrač; co-mentor Igor Mozetič).
- 5. Vid Podpečan, *Knowledge discovery in a service-oriented data mining environment:* doctoral dissertation, Ljubljana, 2013 (mentor Nada Lavrač).
- Branko Jerič, Modeling of teaching based on projects: master's thesis, Nova Gorica, 2013 (mentor Bojan Cestnik).
- 7. Jan Kralj, *A generalization of the Arnoldi algorithm to a nonlinear eigenvalue problem:* master's thesis, Ljubljana, 2013 (mentor Bor Plestenjak).
- Lucija Vidrih, Prospects of lifelong learning at the University of Nova Gorica: master's thesis, Nova Gorica, 2013 (mentor Tanja Urbančič).
- 9. Aljaž Osojnik, *Modeling dynamical systems with data stream mining:* master's thesis, Ljubljana, 2013 (mentor Sašo Džeroski; co-mentor Andrej Bauer).

DEPARTMENT OF INTELLIGENT SYSTEMS E-C

The Department of Intelligent Systems develops new methods and techniques for intelligent computer systems, with applications in the areas of the information society, computer science and informatics, and network communication systems. The main research areas are ambient intelligence, computational intelligence, agent and multi-agent systems, and language and speech technologies. The department collaborates closely with the Faculty of Computer and Information Science of the University of Ljubljana on the joint research program "Artificial Intelligence and Intelligent Systems", led by Prof. Ivan Bratko. The department also collaborates closely with industry and contributes significantly the use of intelligent systems in products and services.

Intelligent systems simulate intelligence so that a typical user perceives them as truly intelligent. In reality, these systems use complex mechanisms and implement them on digital computers to imitate human behavior as well as possible, exploiting raw, exponentially growing computer power.

Ambient intelligence is an increasingly established research area introducing technology into our everyday Head: environment in a friendly way that is undemanding for the user. The two key topics of ambient intelligence we **Prof. Matjaž Gams** work on are (1) telemedicine and elderly care, and (2) smart buildings. On the topic of telemedicine, we successfully completed the European project CHIRON, which is concerned with monitoring chronic heart-disease patients at home. In the past year the project conducted an observational study with real patients, and our department helped analyse the gathered data. We used the CHIRON activity-recognition technology, which utilizes wearable sensors, to win the international EvAAL competition (Evaluating AAL Systems through Competitive Benchmark-

ing). The competition took place in a living laboratory in Velancia, Spain, where an actress performed a sequence of activities, and the competitors had to recognize them with their own equipment. We joined the FP7 project COMMODITY12, which is concerned with monitoring diabetes patients. The role of our department is to analyse the patients' lifestyle with the sensors they use. This means that we will have to recognize their activities and estimate the energy expenditure. While we already have experience with such tasks from the CHIRON project, recognizing high-level activities, such

The department's activity-recognition technology, which uses wearable accelerometers, has won the international EvAAL competition (Evaluating AAL Systems through **Competitive Benchmarking).**

as work, exercise and eating, will be a new challenge for us. Human energy expenditure was estimated with an advanced context-based AI method and presented at the prestigious UbiComp conference. In the ELKOV22 project we collaborate with the Development Center Intech-Les to develop the Intelligent e-Doorman System, which was successfully presented at the Slovenian Innovation Forum. The goal of the system is to utilize intelligent computer methods to offer the services of a human doorman, thus improving the security, comfort and energy efficiency. The e-Doorman is installed on a door with an electro-mechanical lock, sensors, a microcontroller and a tablet computer that serves as the user interface. It uses natural language to communicate with the users, it can learn the users'

habits and automatically recognize them, it can detect break-in attempts and other unusual events, and it has a wide range of additional useful functions. In the past year, three pieces of doctoral research were completed: on the detection of unusual and suspicious behaviour of people, on the detection of diseases of the elderly, and on combining expert knowledge and machine learning (for the purpose of ambient intelligence).

Computational intelligence is a study of stochastic search, optimization and learning methods, inspired by physical and biological systems. Research in this area at the Department of Intelligent Systems focuses on evolutionary computation methods. We study extensions of evolutionary algorithms for multi-objective optimization and their speedup, and apply these algorithms in engineering design and optimization problems. In doctoral research projects, we develop a method for the visualization of multi-dimensional fronts of non-dominated solutions in multi-objective optimization, an algorithm for the discovery of optimal car-driving strategies with respect to the traveling time, fuel consumption and driving comfort, and optimization based on







Figure 2: e-Pedius, a mobile and web application for crowdsourced reassembly of wall paintings

surrogate models. The key areas of testing and transferring our methods to practice are energy efficiency and production process optimization. In collaboration with partners from five European countries, we successfully carried out the 7th Framework Program project MIRABEL (originally MIRACLE). Its goal was to develop a computer infrastructure to efficiently balance between the generation and consumption of electrical energy for an increased amount of energy from renewable sources. The infrastructure relies on flexible offers for energy generation and consumption, their aggregation and scheduling. For this project we implemented scheduling algorithms for assigning the time and energy amount to the offers. We started a new project COPCAMS, accepted for funding under the Artemis call. Together with the Slovenian industrial partner Kolektor and international partners we design quality-control procedures for production that are based on computer vision, machine learning and optimization. In addition, two research projects aimed at optimizing metallurgical production processes are carried out in collaboration with the University of Nova Gorica, the Institute of Metals and Technology, Ljubljana, and the Štore Steel company.

In the field of agent and multi-agent systems the two key topics are agent decision-making architectures and agent-based simulation. The European project ACCUS is aimed at developing an integration and coordination platform for urban systems to build applications across urban systems, provide adaptive and cooperative control for urban subsystems, and to optimize the combined performance. The system

The 7th Framework Program project MIRABEL resulted in a computer infrastructure to efficiently balance between the generation and consumption of electrical energy, and supporting the increasing amount of energy from renewable sources.

will be implemented in Gdansk and Ljubljana. A similar system is studied within the domestic project OPUS, where the focus is on subsystems within a smart house. In the area of agent-based simulation, the project EUSAS is focused on the development of a new approach to mission training for low level units (security, police force, etc.) facing asymmetric threats in an urban environment. The developed tools can be used to discover the common agent strategy by knowing only low-level agent behaviour and possessing basic domain knowledge. The discovered strategic action descriptions are presented to the user in the form of graph paths, agent actions, roles and corresponding rules. Meaningful behaviour

patterns are later used in behaviour cloning, where software agents reproduce the observed human behaviour in a specific domain. The clone is tested in the simulator under all circumstances, thus revealing weak spots and later interactively enabling faster human learning.

In the field of speech and language technologies we work on speech synthesis, semantic analysis of text and question answering. Together with the Amebis company, we develop a new speech synthesizer for Slovene. Special attention is paid to the requirements of elderly, handicapped and visually impaired people. In the past year, we labelled a phonetically rich and balanced speech database for corpus-based speech synthesis using automatic speech-recognition methods. The speech database was recorded in cooperation with the national television and radio, RTV Slovenia. We have established a free text-to-speech conversion service.



Figure 3: Opening of the 16th International Multiconference Information Society - IS 2013 at the Jožef Stefan Institute.

Focus points of developmental and research potential of the department are also being expressed over successfully developed, integrated and deployed solutions, available on major digital platforms and applicable to a wide population of users. The methods used in typical applied projects combine procedures of intelligent agents, statistical methods and machine learning, and they serve as a base for user interfaces on telephones, pads or desktop computers. Projects' services are developed for all key mobile platforms, i.e., Android, iOS, Windows 8 and BlackBerry, and through classic web clients. In the past year, the department obtained and successfully carried out for four innovative projects concerned with the development of e-services and mobile applications for public and private non-profit organizations:

e-Turist (http://www.e-turist.si/) is an application for preparing tourist itineraries adapted to individual users' interests. It takes into account the location, the available time and the opening hours of the attractions. The itineraries are prepared with the help of a recommender system that evaluates the relevance of attractions for each tourist with the help of expert knowledge and the ratings entered in the past by visitors with similar tastes.

The application helps the users to navigate during the trip, and provides them with written and spoken descriptions of the attractions.

e-Asistent (http://www.projekt-asistent.si) is an intelligent assistant capable of communication in natural language that aims to help the user when searching for information on a web page. The assistant platform can be quickly installed on web pages, e.g., of municipalities and of various associations, so that the general base is adapted within a few days to the target content. The service also accepts the user feedback with comments and answer quality, which is in turn assessed and reported to the contracting authority. E-Asistant is implemented at the Slovene

Federation of Pensioners' Associations (ZDUS) and 10 municipalities, the plan in 2014 is to apply it on 100 municipalities. A similar system Svizec is applied at the Education, Science and Culture Trade Union of Slovenia (SVIZ).

e-Pedius (http://e-pedius.si/) is a mobile and web application named after the Roman painter Quintus Pedius. It is a solution that supports crowdsourcing in assembling the fragments of wall paintings. The restoration of wall paintings from fragments of archaeological sites is difficult due to a large number of fragments, their damage and missing parts, hence it usually requires years of manual expert labour. The new solution e-Pedius is accesACCUS smart-city system will design and implement applications for Ljubljana and Gdansk. In a way a similar system OPUS designed for intelligent houses is being developed with the company Robotina. Intelligent control enables a 3 to 20% decrease in costs.

sible to the wider public, including non-specialists, who can use it to reassemble fragments into new compositions, continue the work of other users, and rate the compositions. The solution is designed as a mobile game in which the users gain points for their achievements, and are encouraged to collaborate with other users.

e-Govorec (http://dis.ijs.si/e-govorec) is a mobile application for the voice interpretation of various Slovenian digital texts. The service enables providers with a wide range of e-content to dynamically deliver information in the spoken form of Slovenian language. e-Govorec comes with an integrated synthesizer of speech and is freely available to any user. The application is built with an ear for groups of people with special needs, such as visually impaired and the elderly.

From 7 to 11 October 2013, the 16th International Multiconference Information Society – IS 2013 took place at the Jožef Stefan Institute. It consisted of nine independent conferences with 182 papers. Four conference awards were given: for exceptional contribution to the development and promotion of the information society, for current achievements in the field of information society, and the information strawberry and lemon for the best and worst public information-society services. At the main innovation fair in Slovenia we were the only institution presenting tree systems at the final event.

In 2013, the achievements of the department were 12 times presented on national TV, indicating attractive research and development.

Some outstanding publications in the past year

- 1. Depolli, M., Trobec, R., Filipič, B.: Asynchronous master-slave parallelization of differential evolution for multiobjective optimization. Evolutionary Computation, 21 (2013), 2, 261–291
- 2. Dovgan, E., Javorski, M., Tušar, T., Gams, M., Filipič, B.: Comparing a multiobjective optimization algorithm for discovering driving strategies with humans. Expert Systems with Applications, 40 (2013), 7, 2687–2695
- 3. Kozina, S., Gjoreski, H., Gams, M., Luštrek, M.: Three-layer activity recognition combining domain knowledge and meta-classification. Journal of Medical and Biological Engineering 33 (2013), 4, 406–414
- Gjoreski, H., Kaluža, B., Gams, M., Milić, R., Luštrek, M.: Ensembles of multiple sensors for human energy expenditure estimation. The 2013 ACM International Joint Conference on Pervasive and Ubiquitous Computing, Ubicomp, (2013), 359–362
- 5. B. Kaluža.: Instant Weka How-to. Packt Publishing, 2013

Awards and appointments

1. Matjaž Gams, Hristijan Gjoreski, Simon Kozina, Mitja Luštrek: 1st place at the international activity-recognition competition, EvAAL 2013 (Evaluating AAL Systems through Competitive Benchmarking), Norrköping, Sweden, The AAL Open Association, RAReFall

Organization of conferences, congresses and meetings

- 1. 22nd Slovene Workshop on Nature-Inspired Algorithms, AVN, Šmarna gora, Slovenia, 21. 5. 2013
- 2. 5th Jožef Stefan International Postgraduate School Students Conference, Jožef Stefan Institute, Ljubljana, Slovenia, 23. 5. 2013

- 3. Co-organization of the student workshop at the conference GECCO 2013 (Genetic and Evolutionary Computation Conference), Amsterdam, The Netherlands, 6.–10. 7. 2013
- 4. Workshop for municipalities on the usage of the e-service Asistent, 25. 7. 2013
- 5. Workshop for municipalities on the usage of the e-service Asistent, 26. 9. 2013
- 6. 16th International Multiconference Information Society, IS 2013, 7.-11. 10. 2013; independent conferences:
 - Intelligent systems
 - Facing demographic challenges
 - Collaboration, software and services in information society
 - Cognitive sciences
 - Data mining and data warehouses
 - Education in information society
 - Human-computer interaction in information society
 - Cognitonics
 - Matcos 2013
- 7. Workshop for municipalities on the usage of the e-service Asistent, 18. 11. 2013

Patent granted

- Gregor Černe, Mitja Bizjak, Bogdan Filipič, Tea Tušar, Erik Dovgan, A system for offer selection and request formation in demand response and distributed production of electrical energy, SI24057 (A), Urad RS za intelektualno lastnino, 30.10.2013.
- Matjaž Gams, Rok Piltaver, Erik Dovgan, Andrej Planina, Gašper Pintarič, Bogdan Pogorelc, Intelligent surveillance system and procedure for detection of unusual behaviour, SI23855 (A), Urad RS za intelektualno lastnino, 28.2.2013.

INTERNATIONAL PROJECTS

- 7FP MIRACLE, MIRABEL; Micro-Request-Based Aggregation, Forecasting and Scheduling of Energy Demand, Supply and Distribution European Commission Prof. Bogdan Filipič
- 7FP IntellAct; Inteligent Observation and Execution of Actions and Manipulation European Commission Prof. Matiaž Gams
- 7FP Xperience; Robots Bootstrapped through Learning from Experience European Commission
- Prof. Matjaž Gams
 7FP Commodity12; Continuous Multi-Parametric and Multi-Layered Analysis of Diabetes Type 1&2 European Commission
- Dr. Mitja Luštrek
- EUSAS; European Urban Simulation for Asymmetric Scenarios EADS N.V., Defence and Security Systems Prof. Matjaž Gams

RESEARCH PROGRAM

1. Artificial Intelligence and Intelligent Systems Prof. Matjaž Gams

R&D GRANTS AND CONTRACTS 1. Advanced Modelling and Simulation of Liquid-Solid Processes

- Advanced Modelling and Simulation of Liquid-Solid Processes Prof. Bogdan Filipič
- Simulation and Optimization of Casting, Rolling and Heat Treatment Processes for Competitive Production of Topmost Steels Prof. Bogdan Filipič
- Open Communication Platform for Service Integration: CC OPCOMM Prof. Matjaž Gams
- E-Reader in Slovene for the Blind and Visually Impaired Dr. Tomaž Šef
- Crowdsourcing Support for Reassembly of Wall Painting Fragments Prof. Bogdan Filipič
- Electronic Mobile Tourist Guide Dr. Mitja Luštrek

- 7. Virtual Assistant for Municipalities and Societies Prof. Matiaž Gams
- ARTEMIS, CHIRON; Cyclic and Person-Centric Health Management: Integrated Approach for Home, Mobile and Clinical Environments Dr. Mitja Luštrek
- 9. Adaptive Cooperative Control in Urban (Sub)Systems Prof. Matjaž Gams
- 10. COgnitive & Perceptive CAMeraS: COPCAMS Prof. Bogdan Filipič
- Optimizing the Management of Energy Efficient Smart Buildings Dr. Tomaž Šef
- Research on Adaptive Predictive Domain Models Dr. Boštjan Kaluža

NEW CONTRACTS

- Research of Intelligent Algorithms Applicability for Sensor Data Processing on Embedded Devices Elgoline. d. o. o.
- Prof. Matjaž Gams
- Research of Intelligent Algorithms Applicability for Sensor Data Processing on Embedded Devices Štore Steel, d. o. o.
 - Prof. Bogdan Filipič
- Intelligent Methods for Prediction of Calibration Timing Špica International, d. o. o. Prof. Matjaž Gams
- Analysis and Evaluation of Advanced Spoken Language Technologies for Smart Buildings
- Amebis, d. o. o., Kamnik
- Dr. Tomaž Šef
- 5. Industrial Research aimed at Upgrading the eCampus Learning Management System B2, d. o. o.
- Prof. Bogdan Filipič 6. User-Oriented Business Reporting
- Result. d. o. o.
- Prof. Matjaž Gams
- Critical Analysis and Evaluation of Multiobjective Optimization and Machine Learning Methods for Intelligent Home Services Robotina d. o. o.
 - Dr. Tomaž Šef
- Analysis of Shopping Behavior of Customers in Online Stores Creatim Ržišnik Perc, d. o. o.

VISITORS FROM ABROAD

- 1. Yves Lesteven, University of Paris Sud XI, Paris, France, 7. 4.-6. 7. 2013
- Lucas Drai, Etienne Bohrer, University of Paris Sud XI, Paris, France, 3. 6.–31. 8. 2013
 Martin Gjoreski, Faculty of Computer Science and Engineering, Univerzitet Sv. Kiril in
- Martin Goreski, Faculty of computer Science and Engineering, Univerzitet Sv. Kirli i Metodij, Skopje, Macedonia, 1.–31. 7. 2013

STAFF

Researchers

- 1. Prof. Ivan Bratko*
- 2. Asst. Prof. Aleš Dobnikar*
- Prof. Bogdan Filipič
- 4. Prof. Matjaž Gams, Head
- 5. Dr. Mitja Luštrek
- 6. Dr. Domen Marinčič*
- 7. Dr. Tomaž Šef

Postdoctoral associates

- 8. Dr. Andraž Bežek *, left 01.07.13
- 9. Dr. Matija Drobnič*, left 01.02.13
- 10. Dr. Anton Gradišek
- 11. Dr. Matej Guid*
- 12. Dr. Boštjan Kaluža
- 13. Dr. Aleksander Pivk*
- 14. Dr. Vedrana Vidulin

Postgraduates

- 15. Robert Blatnik, M. Sc.
- 16. Božidara Cvetković, B. Sc.
- 17. Erik Dovgan, B. Sc.
- Tomaž Kompara*, B. Sc.
 Simon Kozina. B. Sc.

BIBLIOGRAPHY

- 4. Ondrej Fikar, Faculty of Electrical Engineering FEL Plzen, Plzen, Czech Republic, 2.-31. 7. 2013
- 5. Wojciech Edward Smietana, Faculty of Computing and Engineering, University of
- Ulster, Belfast, Great Britain, 14. 8.-30. 9. 2013
 Prof. Ronald Sladky, Center for Medical Physics and Biomedical Engineering, Medical University of Vienna, Austria, 7.-11. 10. 2013
- Xavier Labanard, Hadji Bouchelaghem, University of Paris Sud XI, Paris, France, 26. 10. 2013 - 5. 1. 2014
- 20. Dr. Jana Krivec*
- 21. Damjan Kužnar, B. Sc.
- 22. Dr. Violeta Mirchevska
- 23. Miha Mlakar, B. Sc.
- 24. Rok Piltaver, B. Sc.
- 25. Dr. Bogdan Pogorelc, left 01.09.13
- 26. Aleš Tavčar, B. Sc.
- 27. Tea Tušar, M. Sc.
- 28. Jernej Zupančič, B. Sc.
- Technical officers
- 29. *Mitja Kolbe*, B. Sc., left 01.07.13* 30. Blaž Mahnič, B. Sc.
- Gašper Pintarič*, B. Sc.
- Technical and administrative staff
- 32. Vesna Koricki Špetič, B. Sc.
- 33. Mitja Lasič
- 34. Liliana Lasič
- 35. Lana Zemljak

Note: * part-time JSI member

ORIGINAL ARTICLE

- 1. Marko Bohanec, Martin Žnidaršič, Vladislav Rajkovič, Ivan Bratko, Blaž Zupan, "DEX methodology: three decades of qualitative multi-attribute modeling", *Informatica (Ljublj.)*, vol. 37, no. 1, pp. 49-54, 2013.
- Božidara Cvetković, Boštjan Kaluža, Radoje Milić, Mitja Luštrek, "Towards human energy expenditure estimation using smart phone inertial sensors", In: Ambient intelligence: 4th International Joint Conference, AmI 2013, Dublin, Ireland, December 3-5, 2013: proceedings, *Lect. Notes Comput. Sci.*, vol. 8309, pp. 94-108, 2013.
- Božidara Cvetković, Simon Kozina, Boštjan Kaluža, Mitja Luštrek, "Energy expenditure estimation DEMO application", In: Ambient intelligence: 4th International Joint Conference, AmI 2013, Dublin, Ireland, December 3-5, 2013: proceedings, *Lect. Notes Comput. Sci.*, vol. 8309, pp. 281-286, 2013.
- Matjaž Depolli, Roman Trobec, Bogdan Filipič, "Asynchronous masterslave parallelization of differential evolution for multiobjective optimization", *Evol. comput.*, vol. 21, no. 2, pp. 261-291, 2013.
- Sara Dolci, Vincenzo Ieraldi, Anton Gradišek, Zvonko Jagličić, Maja Remškar, Tomaž Apih, Mario Cifelli, Guido Pampaloni, Carlo Alberto Veracini, Valentina Domenici, "Precursors of magnetic resonance imaging contrast agents based on cystine-coated iron-oxide nanoparticles", *Current physical chemistry*, vol. 3, no. 4, pp. 493-500, 2013.
- Erik Dovgan, Matija Javorski, Tea Tušar, Matjaž Gams, Bogdan Filipič, "Comparing a multiobjective optimization algorithm for discovering driving strategies with humans", *Expert syst. appl.*, vol. 40, no. 7, pp. 2687-2695, 2013.
- Bogdan Filipič, Risto Vesanen, Erkki Laitinen, "Scalar vs. vector approach to bi-objective resource allocation in spatially distributed networks", *International journal of innovative computing and applications*, vol. 5, no. 3, pp. 191-197, 2013.
- Iztok Fister, Marjan Mernik, Bogdan Filipič, "Graph 3-coloring with a hybrid self-adaptive evolutionary algorithm", *Computat. optimiz. appl.*, vol. 54, iss. 3, pp. 741-770, 2013.
- 9. Matjaž Gams, "Alan Turing, Turing machines and stronger", *Informatica (Ljublj.)*, vol. 37, no. 1, pp. 9-14, 2013.
- Anton Gradišek, Tomaž Apih, Valentina Domenici, Vladimíra Novotná, Pedro J. Sebastião, "Molecular dynamics in a blue phase liquid crystal: a

¹H fast field- cycling NMR relaxometry study", *Soft matter*, vol. 9, no. 45, pp. 10746-10753, 2013.

- 11. Anton Gradišek, Dorthe Ravnsbæk, Stanislav Vrtnik, Andraž Kocjan, Janez Lužnik, Tomaž Apih, Torben R. Jensen, Alexander V. Skripov, Janez Dolinšek, "NMR study of molecular dynamics in complex metal borohydride LiZn₂(BH₄)₅", *The journal of physical chemistry. C, Nanomaterials and interfaces*, vol. 117, no. 41, pp. 21139-21147, 2013.
- 12. Vida Groznik, Matej Guid, Aleksander Sadikov, Martin Možina, Dejan Georgiev, Veronika Kragelj, Samo Ribarič, Zvezdan Pirtošek, Ivan Bratko, "Elicitation of neurological knowledge with argument-based machine learning", *Artif. intell. med.*, vol. 57, no. 2, spec. iss., pp. 133-144, 2013.
- Matej Guid, Ivan Bratko, "Search-based estimation of problem difficulty for humans", In: Artificial intelligence in education: AIED 2013: 16th International Conference, Memphis, TN, USA, July 9-13, 2013: proceedings, *Lect. Notes Comput. Sci.*, vol. 7926, pp. 860-863, 2013.
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DEPARTMENT OF REACTOR ENGINEERING

R-4

The Department of Reactor Engineering is involved in basic and applied research in the fields of nuclear engineering and safety. Topics include the modelling of basic thermal-hydrodynamic phenomena, thermal-hydraulic safety analyses of design-basis and severe accidents, structural safety analyses and probabilistic safety assessments. Most research activities are part of international cooperation programs. The research results are incorporated in projects for industry and for the regulatory authorities, as well as in undergraduate and doctoral studies programmes.

Modelling of basic thermal-hydrodynamic phenomena

Research on turbulent heat transfer was continued. A theoretical analysis of a heated slab cooled with a turbulent flow on both sides was performed using Direct Numerical Simulation. The results predict a penetration of the turbulent temperature fluctuations into the solid wall. For a sufficiently thick slab, temperature fluctuations from both sides of the slab do not interfere. However, as the slab gets thinner, fluctuations from both sides interfere and tend to a finite value as the slab thickness limits towards zero. The research was related to the THINS project (7th European Commission Framework Programme) and might be relevant for next-generation fission reactors that will be cooled with liquid metals.

Simulations of turbulent flow in a horizontal fuel bundle with mixing vanes were continued (OECD/NEA benchmark), using an open-source code. Computational analyses were focused on improvements to the turbulence modelling and computational grid, and were verified with the MATIS-H experiment (Measurement and analysis of turbulent mixing in sub-channels – horizontal) that was performed at KAERI (Korea Atomic Energy Research Institute) in South Korea.

For the past few years, the department has been actively involved in the development of a helium-cooled diverter for the DEMO fusion reactor. Heat removal by multiple jet impingement is foreseen for divertor cooling. Turbulent

flow structures that are generated in the area where the jets impinge on the cooled surface are crucial for effective cooling. The formation and propagation of the structures, and their influence on the local heat-transfer characteristics were analysed numerically by means of a Large Eddy Simulation, in cooperation with the Paul Scherrer Institute (Switzerland).

Research on numerical methods in fluid mechanics was continued as well. In the frame of the NURESAFE project (7th EC FP), new theoretical models for interface capturing and sharpening within two-fluid models of two-phase flow were examined. The simulation of a simple air-water counter-current flow, related to so-called flooding in vertical pipes, was carried out. Detailed knowledge of basic physical mechanisms of the flooding phenomena in pipes is of particular interest for safety analyses of a loss-of-coolant accident in nuclear reactors.

Natural convection in a closed cavity was analysed with various versions of spectral schemes that are used to solve numerically the transport equations of fluid mechanics, as well as with the Lattice-Boltzmann method. Various runs were performed to test the accuracy of the numerical schemes and the efficiency of the parallelization on parallel computers.

Basic phenomena that might occur during a hypothetical severe accident in a nuclear power plant were investigated. A steam explosion is an energetic fuel-coolant interaction process, which may occur if, during an accident, the hot reactor-core melt comes into contact with coolant water. Steam explosions are an important nuclear safety issue because they can potentially jeopardize the primary system and the containment integrity of a nuclear plant. Within the SERENA project (OECD/NEA) and the SARNET2 network (7th EC FP), we continued simulations and analyses, using the European code MC3D, of steam explosion experiments performed in the KROTOS (Commissariat à l'Energie Atomique - CEA, France) and TROI (KAERI) facilities. Based on the developed single-melt droplet-solidification model, fragmentation A new method for the assessment of the on-site power system reliability after an earthquake with a specific magnitude was developed.



Figure 1: Large Eddy Simulation (LES) of multiple impinging jets: vortical structures (left) and profiles of the local heat-transfer coefficient at the cooled surface (right) are presented in two characteristic planes.

criteria for fuel-coolant interaction codes were established for various non-eutectic prototypic materials. Both singleand multiple-droplet size group modelling approaches were considered. The important influence of the metallic



is

zirconium content in prototypic oxidic corium on the steam explosion energetics was analysed using SERENA and ZREX (Argonne National Laboratory, USA) experimental results. To explain the observed experimental behaviour,

Using Direct Numerical Simulation, we have analysed the penetration of temperature fluctuations into the interior of a hot slab cooled on both sides by flowing liquid. the hydrogen film hypothesis was proposed. A comprehensive oxidation influence study was performed with the MC3D code, which supports the proposed hypothesis. Apart from that, the potential of strong vapour explosions during melt-sodium interaction was investigated as well.

In the field of modelling of atmosphere mixing in the containment, we have simulated the experiment NATHCO that was performed in the MISTRA

facility (CEA) within the SETH-2 project (OECD/NEA). The simulation successfully replicated the natural circulation in the MISTRA vessel, which was induced by gradual heating of the vessel walls. The influence of two different models of turbulence was also compared.

Thermal-hydraulic safety analyses

Stress tests, which had to be performed in European nuclear power plants after the accident at the Fukushima Daiichi (Japan) nuclear power plant in 2011, also required an evaluation of the consequences of the loss of safety functions due to station blackout (SBO). Therefore, long-term SBO analyses of a two-loop pressurized water reactor (PWR) were performed using the RELAP5/MOD3.3 computer code to evaluate the time before the water level reaches the top of the reactor core and the time of significant core heat-up. Different reactor coolant pump (RCP) seal leaks were assumed, using two main strategies: depressurization of the reactor coolant system (RCS) and water injection into RCS. The results suggest that for the expected magnitude of RCPs seal leaks in the selected two-loop PWR, the core uncovery during the first seven days could be prevented by an available turbine-driven auxiliary pump (TD AFW) and manually depressurizing the RCS through the secondary side depressurization. In scenarios without TD



Figure 2: Fluid temperature fields at the inner pipe wall emulating thermal loads downstream of a T-junction for a turbulent mixing of hotter (200°C) and colder (100°C) water: a) calculated temperature fluctuations, b) provided mean temperatures, c) final temperatures.

AFW pumps, the core uncovers and heats up in less than one week. The experiment on hydrogen combustion that was performed in 2012 in the HYKA A2 facility at the Karlsruhe Institute of Technology (Germany) was simulated with the lumped-parameter code ASTEC. The HYKA A2 facility is a cylindrical vessel with a volume of 240 m³. A hydrogen-steam-air mixture was ignited at the bottom of the vessel, which caused combustion and flame propagation in the vertical and radial directions. An international benchmark exercise for lumped-parameter codes was also organised, with contributions from RSE (Italy), UJD SR (Slovakia), NUBIKI (Hungary), LEI (Lithuania) and JSC Atomenergoproekt (Russia).

For the case of a spent-fuel-pit (SFP) accident, a calculation procedure was developed, which, based on monitoring of either the coolant level elevation, or leakage intensity, or dose rate on the edge of the SFP, assesses the pool integrity indirectly. Once the crack of the SFP has been characterized in terms of the size and the vertical location of the rupture, the procedure presents the necessary and possibly the only means for predicting the course of an extreme event. During the remediation of the damage, these data can be used for assigning the priorities, optimizing absorbed doses and eventually for anticipating the timely evacuation of the site.

Structural safety analyses

Recent research has been focused on the development of multiscale computational simulation tools for polycrystalline metallic materials. An advanced constitutive model of crystal plasticity is combined with random grain sizes and shapes. The data on crystal grains are retrieved either from experimental (e.g., X-ray diffraction contrast tomography) or analytical (e.g., Voronoi tessellation) methods. The loading of randomly shaped and oriented crystal grains with anisotropic properties results in highly inhomogeneous microscopic stress fields, which are estimated using the finite-element solver ABAQUS.

In 2013 we introduced and compared cohesive-element and cohesive-zone approaches to modelling the intergranular cracking on the grain level. The cohesive-surface approach proved to be simpler to implement, while the cohesive elements made the tracking of the damage initiation and evolution easier. In addition, the cohesive-surface approach proved to be numerically much more stable compared to cohesive elements. To alleviate the convergence issues, we developed an analytical expression for assessing the cohesive element response when using viscous regularization. The development of the simulation method benefits from our collaboration with the EC Joint Research Center in Petten (Netherlands).

We calibrated a crystal-plasticity finite-element model to describe the deformation behaviour of single-crystalline 316L stainless steel. This type of steel is an important structural material used for in-core components and pressure boundaries of light water reactors. Nine hardening

parameters were identified by fitting the calculated stress-strain curves to corresponding measurements in three tensile directions. A very good agreement with the measurements was found in all directions.

Regarding thermal fatigue research, a new approach was developed for the fast and reliable generation of random surface thermal loads which relies on the approximation of fluid temperature fluctuations with the linear superposition of plane waves. The approach employs fluid temperature statistics, such as the mean and variance, from experimental or computational simulations results. The approach was applied to fatigue analyses of pipes.

We have also addressed the structural integrity of PWR fuel rods by employing the hydration effects of Zircalloy-4 cladding tubes during in-service operation. A finite-element model of the fuel rod was developed for different hydride blister morphologies. A damage model for the cladding was constructed and analysed in comparison with experimental results.

Part of the work was related to international research projects. Within the MULTIMETAL (7th EU FP) project, we performed finite-element calculations of the fracture toughness for several pre-cracked specimen designs. In the bilateral project with CEA, the realistic stainless-steel wire model was modified to suit the CEA finite-element code Castem.

Probabilistic safety assessment

A new method for the assessment of the on-site power system's reliability after an earthquake with a given magnitude was developed. The new method considers the design features and functional dependencies within the

on-site power system and the seismic fragility of the constituting elements. The obtained results show the importance of the on-site power system's reliability in general and battery supported section of the Class 1E power system in particular for the safety of the nuclear power plant. A high level of reliability is obtained for the Class 1E and Non-1E power system during normal operation and safe shutdown during an earthquake. The calculated

A new approach was developed for the fast and reliable generation of continuous temperature fields that emulate thermal loads in T-junction piping due to turbulent fluid mixing.

results show a high level of reliability of a Class 1E power system after an earthquake with peak ground acceleration equal to the one measured at the Fukushima Daiichi (Japan) nuclear power plant during the 2011 earthquake. A revision of the current guideline for assessment of the acceptable station blackout duration capability was recommended, considering the results of the analysis and identified deficiencies in the current guideline.

A new model for the optimal generation dispatch of a power system was proposed. The model extends the classical combined economic-environmental power dispatch considering the availability of the generating units as the third objective. The unavailability of power generation is defined as the risk index and is considered to be a function of the generating units' power level. The results show an increase of the availability of power generation followed by a small increase in the fuel costs and the gaseous emission.

The Slovenian power system was analysed using a multi-objective generation scheduling model. The model considers three objective functions: fuel costs, emissions of gaseous pollutants and unavailability of power generation. First, the conventional generation scheduling is solved taking into consideration only the fuel costs. Second, the generation scheduling is solved as a combined risk-economic-environmental optimization problem that takes into consideration all the above-mentioned objectives. The results show that smart scheduling of power generation may decrease the emissions and increase the availability of power generation in the Slovenian power system.

Technical cooperation, consulting services and education

Reactor Engineering Department researchers also cooperated in projects for industry. As an authorized institution for radiation and nuclear safety, and in the framework of regular Krško nuclear power plant (NPP) activities for maintenance and improvements to nuclear safety, we performed an independent expertise of the regular Krško NPP outage. During the outage, we performed inspection activities on safety structures, systems and components. A report with proposals for safety improvements was prepared.

Apart from that, the Reactor Engineering Department was contacted by the Krško NPP to perform a part of the review in the framework of the 2nd Periodic Safety Review (PSR). The PSR is a comprehensive safety review of all the important aspects of safety and is carried out at regular intervals (typically 10 years). The PSR is subdivided into 14 safety factors. We performed a review of three safety factors: deterministic safety analyses, probabilistic safety analyses and hazard analyses. Separate reports on each of the safety factors were prepared with proposals for safety improvements.

Members of the department are also actively involved in nuclear engineering under-graduate, master and doctoral studies at the Faculty of Mathematics and Physics at the University of Ljubljana. The programmes are associated with the European Nuclear Education Network (ENEN) and the European project ENEN-III.

Organization of conferences, congresses and meetings

- 1. International conference NENE2013 "22nd International Conference Nuclear Energy for New Europe", Bled, Slovenia, 9. 9.–12. 9. 2013
- 2. Regional meeting of NEWLANCER, Ljubljana, Slovenia, 15.-17. 4. 2013
- 3. Autumn meeting of users and administrators SLING, Ljubljana (JSI Reactor Center), Slovenia, 13. 11. 2013

INTERNATIONAL PROJECTS

- 7FP SARNET2; Network of Excellence for a Sustainable Integration of European Research on Severe Accident Phenomenology and Management - Phase 2 European Commission Dr. Matjaž Leskovar
- 7FP EURATOM ENEN-III; European Nuclear Education Network Training Schemes European Commission Prof. Leon Cizelj
- 7FP EURATOM THINS; Thermal-hydraulics of Innovative Nuclear Systems European Commission Prof. Iztok Tiselj
- 7FP EURATOM TRASNUSAFE; Training Scheme on Nuclear Safety Culture European Commission
- Prof. Borut Mavko5. 7FP NEWLANCER; New MS Linking for an Advanced Cohesion in Euratom Research European Commission
- Prof. Leon Cizelj
 7FP EURATOM; MULTIMETAL; Structural Peformance of Multi-metal Component European Commission
- Prof. Leon Cizelj 7. 7FP - NURESAFE; Nuclear Reactor Safety Simulation Platform European Commission
- Dr. Boštjan Končar
- 7FP CESAM; Code for European Severe Accident Management European Commission Asst. Prof. Ivo Klienak
- 7FP ASAMPSA_E; Advanced Safety Assessment: Extended PSA European Comprision
- European Commission Dr. Andrija Volkanovski 10. 7FP - ARCADIA: Assessment of Regional Capabilities
- 7FP ARCADIA; Assessment of Regional Capabilities for New Reactors Development through an Integrated Approach European Commission
- Prof. Leon Cizelj
- 7FP EURATOM, Public Information; Research Unit Administration and Services RU-FU; 3211-08-000102, FU07-CT-2007-00065 Ministry of Education, Science and Sport
- Dr. Boštjan Končar 12. 7FP - EURATOM, MHEST Association; Divertor High Flux Helium Cooling - 4.5.1. - FU, FU-07-CT-2007-00065 Ministry of Education, Science and Sport
 - Dr. Boštjan Končar
- 13. 7FP MHEST Association EURATOM, 4.10.1.-FU; TH Analyses of DEMO Blanket Ministry of Education, Science and Sport
- Dr. Boštjan Končar 14. 7FP - EURATOM-MHEST; WP13-DAS-02-T12-01/MESCS/PS, Helium Cooled Divertor Design and Fabrication Analysis
- Ministry of Education, Science and Sport Dr. Boštjan Končar
- Training and Tutoring for Experts of the NRAs and their TSOs for Developing and Strengthening their Regulatory and Technical Capabilities - INSC Project MC.03/10 -LOT 1: Training and Tutoring for Nuclear Regulatory Authorities and their TSO's ITER-consult Srl Prof. Leon Cizelj
- Investigation of Flow Boiling Mechanisms in Nuclear Engineering Slovenian Research Agency Dr. Boštian Končar

VISITORS FROM ABROAD

- Prof. Hiroshige Kikura, Tokyo Institute of Technology, Department of Nuclear Engineering, Tokyo, Japan, 25. 2. 2013
- Dr. Imre F. Barna, Centre for Energy Research of the Hungarian Academy of Sciences, Budapest, Hungary, 26.–30. 8. 2013
- Ricard Mas Fillol, Universitat Politecnica de Catalunya (UPC), Barcelona, Spain, 18. 2.–30. 9. 2013

- European Nuclear Society; ENS Board of Directors; ENS High Scientific Council Meeting Slovenian Research Agency Prof. Leon Cizelj
- SNETP Sustainable Nuclear Energy Technology Platform; SNETP General Assembly Slovenian Research Agency Prof. Leon Cizeli
- Application and Validation of Multiscale Method for Two-phase Flow Analyses in Nuclear Reactors
 - Slovenian Research Agency Dr. Boštjan Končar
- Dividing of Atmosphere Stratification Breakup Experiments with Lumpedparameter Codes Slovenian Research Agency
- Asst. Prof. Ivo Kljenak
- Comprehensive and Reliable Prediction of LWR's Internals Mechanical Behavior Based on Microstructure-informed Modeling Slovenian Research Agency
- Dr. Samir El Shawish
- 22. Influence of Oxidation and Large Solidification Temperature Range of Fuel Coolant Interaction Slovenian Research Agency
 - Dr. Matjaž Leskovar

RESEARCH PROGRAM

1. Reactor engineering Prof. Leon Cizelj

R&D GRANTS AND CONTRACTS

- 1. Experiment and Simulation of Hydrogen Combustion in Nuclear Power Plant Containment Experimental Facility Prof. Borut Mavko
- Development of Methods and Models for Simulation of Thermal-Hydraulic Phenomena in Innovative Nuclear Reactors Prof. Iztok Tiselj
- Steam Explosions in Sodium Cooled Fast Reactors Dr. Mitia Uršič
- Code Applications and Maintenance Program (CAMP); Thermal-Hydraulic Code Applications and Maintenance Dr. Andrej Prošek

NEW CONTRACTS

- Cooperation in an International CAMP Program Krško Nuclear Power Plant Dr. Andrei Prošek
- Expert Opinion in Krško NPP Tests and Repairs During Refuelling 2013 Milan Vidmar Electroinstitute Liubo Fabian. M. Sc.
- 4. Prof. Grzegorz Wrochna, National Centre for Nuclear Research, Swierk, Poland, 13. 9. 2013
- Dejan Židan, M. Sc., Ministry of Agriculture and the Environment, Ljubljana, Slovenia, 13. 8. 2013
- Prof. Ivo Roghair (with students), Eindhoven University of Technology, T.S.V. 'Jan Pieter Minckelers', Eindhoven, Netherlands, 7. 11. 2013

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REACTOR INFRASTRUCTURE CENTRE

RIC

The Reactor Infrastructure Centre incorporates a research reactor TRIGA Mark II Reactor and a Hot Cells Facility. The reactor, operating since 1966, is used for neutron research, training and producing radioactive isotopes. A detailed technical description of the reactor is available at http:// www.rcp.ijs.si/~ric/. The Hot Cells Facility is used for the treatment and handling of radioactive materials and radioactive waste within research and applicative projects. In addition, it is used for performing measurements within the regular radiological monitoring of the reactor.

Besides operating and maintaining the reactor, the members of the reactor staff participate in other activities requiring specialists skilled in work with sources of radiation and in reactor technology, such as the servicing of industrial radioactive sources and surveillance of the fuel management in NPP Krško.

In 2013 the reactor operated for 136 days. Altogether, 825 samples were irradiated in the rotary specimen rack and 16 in the pneumatic transfer system. There were no serious operational problems or events influencing nuclear or radiation safety. The reactor operators were performing regular maintenance inspections and activities according to the annual plan.

In the Hot Cells Facility the activities were mostly performed by the Department of Environmental Sciences and the Radiation Protection Unit. The IJS staff performed training in radiochemistry and radioactivity measurements for practitioners from countries eligible under the JRC Enlargement & Integration policy. The treatment and conditioning of low and intermediate radioactive waste for subsequent storage in the central storage for radioactive waste was continuously performed together with the Slovenian Agency for Radioactive Waste Management (ARAO).

The reactor was mainly operated for the needs of the Jožef Stefan Institute's Nuclear Training Centre, for educational purposes (Faculty of Mathematics and Physics, University of Ljubljana and Faculty for Energy, University of Maribor) and research departments: Environmental Sciences, Reactor Physics and Experimental Particle Physics. The reactor was used for the following research:

- Reactor physics and neutronics,
- Activation analysis,
- · Research on radiation damage of semiconductors,
- Neutron dosimetry and spectrometry,
- Neutron radiography,
- · Activation of materials, nuclear waste and decommissioning,
- Irradiation of materials for fusion reactors,
- Irradiation of electronic and medical components,
- Development and testing of new detectors,
- Development of new methods for measuring power profiles, neutron spectra, etc.,
- Verification and validation of methods for calculating the transport of neutrons, photons and electrons,
- Development of educational tools in reactor physics.

The TRIGA reactor participates in the FP7 AIDA (Advanced Infrastructures for Detectors and Accelerators) project that brings together advanced European infrastructures for future particle-physics experiments.

Within the frame of the "Experimental Verification of Kinetic Parameters of the TRIGA Reactor and the Upgrade of the Digital Meter of Reactivity" some experiments we conducted.

The project "Thermal neutron irradiation testing of NI PXI and cRIO products" together with National Instruments and ITER organization including the irradiation and testing of electronic instruments was brought to the end.

Within the international collaboration with the CEA, France, we tested the resistance of polyethylene capsules to thermal neutrons (project Design of an irradiation device for FT-TIMS method at the JSI TRIGA Mark II reactor) and performed preliminary measurements of the fission and ionisation chambers' response (project name: experimental verification of flux form factors and qualification of wide range neutron instrumentation).

In collaboration with the reactor physics division and CEA France a series of experiments were performed in order to determine the kinetic parameters of the reactor. This was the first time the measurements were performed with four fission chambers simultaneously. In addition, the new CEA developed system, called SPECTRON, was tested. Within the framework of this project the control rod worth measurement methods were improved. In another



Prof. Borut Smodiš

CEA project the IRDFF dosimetry library was tested by the rector physics division and CEA. The calculations were compared against activation measurements at the TRIGA reactor in order to accurately determine the neutron spectra and irradiation channels.

The projects within the framework of the IAEA Technical Coordination Programme entitled "Carrying out a Feasibility Study and Installing the Thermal Neutron Driven 14 MeV Neutron Converter into the TRIGA Research Reactor" and the Installation of DT converter of neutrons in the TRIGA reactor" was continued.

Within the framework of the contract "Irradiation and Analysis for Si samples" with the Institute of Radiation



Figure 1: Last year we had bubbles in the reactor, this year we have a reactor inside the bubbles.

Problems of AzNAS, Azerbaijan, various samples were irradiated in the TRIGA reactor and analysed in cooperation with some JSI departments. The project will continue in 2014.

The collaboration with INMEDICA, Slovenian Device Incubator for Medical Systems and Treatments was established, in the frame of which medical equipment is irradiated and the changes after irradiation are observed.

Practical exercises in reactor physics and kinetics for the students of physics at the University of Ljubljana were performed. Some of the exercises were performed for the first time in the history of the reactor.

The work on the Periodic Safety Report, that started in 2011, continued. The reactor operators took part at the outage of NPP Krško.

Before the reactor start-up at the NPP Krško, preparations and tests to conduct physical tests took place at the TRIGA reactor.

The reactor operators supported the researchers by performing the operations and services for which the researchers are not qualified and authorized, such as operating the reactor, performing irradiations and manipulating radioactive samples.

The research results were published in approximately 20 scientific papers. Seven young researchers performed their research at the reactor.

In November 2012 an IAEA INSARR mission was conducted. The objective of the mission was to review the operational safety of the reactor, including reactor management and regulatory supervision, Safety Analysis Report, safety analyses, Operational Limits and Conditions, conduct of operations, maintenance, training and qualifications of the operating personnel, utilization and modifications, operational radiation protection and waste management, emergency planning, quality assurance and decommissioning plan. The work on recommended issues was carried out in 2013 and continued in 2014.

In 2013 the following international course in the field of the safety of research reactors was performed: 1.

TJET14: Nuclear Power Plant Technology, ICJT, 5.11.-2012 -. 5.4.2013, 22 participants.

Practical exercises in reactor physics and kinetics for the students of physics at the University of Ljubljana were preformed. The postgraduate students of nuclear engineering attended some of these exercises as well. For these purposes the reactor operated for approximately 2 months. The reactor was also used for practical exercises within the training program of the NPP Krško reactor operators. The exercises were prepared and carried out by the reactor personnel in co-operation with the Nuclear Training Centre and the Department of Reactor Physics. In 2013, there were more than 50 short group visits to the reactor. The visitors were mainly foreign scientists, students and more than 33 groups of school children. The total number was more than 900.

INTERNATIONAL PROJECTS

Reports on Thermal Neutron Induced SEU Susceptibility of PXIe and cRIO Fast 1. Controller Components ITER Organization

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Dr. Luka Snoj
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- Training in Radiochemistry and Radioactivity Measurements for Practitioners from 2 Countries Eligible under the JRC Enlargement & Integration Policy Institute for Reference Materials and Measurements Prof. Borut Smodiš
- Feasibility Study and Installation of Thermal Neutron Driven 14 MeV Neutron Converter 3. into the TRIGA Research Reactor IAEA - International Atomic Energy Agency
 - Dr. Luka Snoi
- NATO SPS.EAP.SFP 984524; Radioactive and Heavy Metal Waste Tailings Risk Reduction in Fergama Valley, Kyrgyz Republic NATO - North Atlantic Treaty Organisation Prof. Peter Stegnar

- Automation of a Pneumatic Transport System for Neutron Activation Analysis IAEA - International Atomic Energy Agency Prof Borut Smodiš
- 6 Training Fee for Ms Ilona Matveveva, (Kazakhstan), 1, 6, 29, 8, 2013 ICTP - Centro Internazionale di Fisica Teorica Prof Borut Smodiš

R&D GRANTS AND CONTRACTS

- Calculations to Support Neutron Monitor Calibration JET Fusion Reactor Example Case 1. Dr. Luka Snoj
- 2 Small Services in Year 2013 Foreign Clients Dr. Luka Snoj
- 3. Irradiation and Analysis of Si Samples Anže Jazbec, B. Sc.

NEW CONTRACT

 Treatment and Conditioning of Radioactive Waste for Storage ARAO Prof. Borut Smodiš

STAFF Researchers

Prof. Borut Smodiš, Head
 Dr. Luka Snoj
 Postgraduate
 Anže Jazbec, B. Sc.
 Technical officer
 Dr. Tinkara Bučar

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- Darko Kavšek, B. Sc.
 Marko Rosman
- 8. Sebastjan Rupnik, B. Sc.

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NETWORKING INFRASTRUCTURE CENTRE NIC

The Networking Infrastructure Centre (NIC) is responsible for the administration, development, management and expansion of the core network and ICT services and infrastructure for the Jožef Stefan Institute. It also provides the development of computing, communication, data and security infrastructure for the research departments, centres and services of the Institute.

The NIC's main mission is to provide a high level of connectivity and integration to the local and international communication networks and infrastructures for research departments, programmes, groups and projects and to provide ICT support for the research activities at the Jožef Stefan Institute, including the development, management and administration of the ICT and computing infrastructure, technology, facilities and services at the institute. We work in four main domains: networking infrastructure, network security, network services and distributed network computing.

Networking infrastructure. The Networking Infrastructure Centre provides development, management,

administration and support to the physical networking infrastructure for the institute and support to local networks Head: so as to enable internal and internet connectivity to the users and services at the Institute. The institute network Vladimir Alkalaj, M. Sc.*

includes its wireless networks and a number of dedicated networks for specific services, projects and activities (i.e., dedicated links to other institutions, secure links to the Reactor Infrastructure Centre Podgorica etc.). *Physical network:* Due to the increased requirements of several research groups and organizational units, our physical network has been extended and

optimized in the past year. A number of core backbone routing and switching upgrades enabled us to provide higher throughput and lower latency as well as expanding the network and its support for IPv6.

In the course of the ongoing upgrading of the physical network infrastructure at the Reactor Infrastructure Centre Podgorica, the physical link to the RIC site has been upgraded with a 10 Gbit/s capacity, which makes it possible to implement multiple dedicated managed VLAN connections and fully integrate the RIC network with the core network at the Institute's main campus. A number of local active switching equipment units have been upgraded to facilitate access to the faster backbone and support newer protocols.

An additional external 10 Gbit/s connection via the ARNES and GÉANT networks has been established with the dedicated LHCONE network (LHC Open Network Environment) to support the high network throughput demands of the ATLAS project inside the WLCG (Worldwide Large Hadron Collider Computing Grid) Nordic computing cloud. The new link replaced the dual 1 Gbit/s links and lessened the load on the Institute's main uplink, the ARNES international links and the Nordic NREN's international links. Internally, we have implemented a redistribution between the relevant OSPF area and the BGP, used on the LHCONE network, enabling us to easily implement additional dedicated international connections (also known as light-paths).

Monitoring: We have implemented a new traffic- and status-monitoring infrastructure based on the free software package Observium, which allows us to respond dynamically to changes in usage and traffic in the context of the Institute's network. We have developed a new system for environmental monitoring, assisting us in the design of higher density racks in the computing centre, while minimising any equipment damage due to overheating. Figure 1: Observium: a view of the daily traffic at a network switch The new system includes our own design of micro-controller-enabled sensors

A network backbone with new routers and an upgraded 10 Gbit/s link to the Reactor Infrastructure Centre Podgorica, an additional external dedicated 10 Gbit/s link, BGP support and increasing Wi-Fi AP numbers are just some markers of the rapid network expansion at the Jožef Stefan Institute.



and firmware. The development and deployment was cheaper than purchasing comparable commercial offerings and it replaced our previous solution that used "single wire" sensors with a new one based on the CAN bus, used in industrial and vehicle design, with higher tolerance, longer permissible distances (100 m+ link length) and the possibility to connect more than a hundred sensors to a single bus. The units carry dual temperature sensors to improve the measurement quality and a zero-power-based microcontroller to minimise any measurement drift due *Photo by Sašo Radelj

to the sensors' own power use. All the sensors are synchronically calibrated and therefore quite accurate. We use an accuracy of 0.1 °C while the maximum accuracy is stated at 0.02 °C. An in-house firmware and driver solution allows the integration with standard protocols (SNMP) and interoperability with existing monitoring systems, including Observium.

Wireless network: Due to a rapid increase in the number of wireless clients (more users with more devices), we have continued with the deployment of new wireless access points in order to improve on the useful signal density and coverage of the institute's wireless network. We have also completed the testing of wireless network control modules to improve security and introduce wireless network segmentation.

IPv6 support: Due to upgrades and improvements in the core network router protocol support, the active equipment now offers better SNMP protocol support over the IPv6 protocol stack, allowing us to implement network monitoring and administration without the use of the IPv4 stack, thus alleviating the load on the already mostly spent IPv4 address pool. We have been testing a new firmware revision for wireless access points that provides an implementation of the RADIUS authentication over the IPv6 stack, which is already supported in the open source FreeRADIUS package in version 3. The IPv6 protocol family, already fully supported in our public services and user-accessible service, is now also fully usable for internal services and tasks.

Network Security. The NIC is responsible for implementing security measures and policies in three domains: external network connectivity security, security of the network itself and security of the services and software deployments.

External network security is provided with the dynamic management and configuration of deep packet inspection firewall systems and routing configuration, with the exception of dedicated links where passive measures (configuration, filtering and supervision) are used. Security policy and the implementation of the institute network

The internal development of e-mail security and filtering, active network firewalling, introduction of cryptography and certification and close collaboration in national and international security response centres and networks are the basis of an open academic network in the age of the hostile Internet. is very complex due to the requirements of an open academic network that collide with current security considerations due to the increased detection of threats from the outside network. Therefore, ensuring the secure and open environment requires disproportionate increases in equipment capabilities and efforts in the dynamic security policy configuration.

Since the NIC is responsible for the security of the ICT infrastructure of the Institute, we are active members of relevant institutions and groups, notably the national security response centre SICERT, FIRST (Forum of Incident Response and Security Teams), EGI CSIRT (European Grid Initiative

distributed computing security incident response team), we are part of the response team of the national distributed computing network SLING. The national science certificate agency SiGNET CA, managed by the NIC, is a full member of EU Grid PMA (EU Grid Policy Management Authority) and IGTF (Internet Grid Trust Federation). We have participated in the creation of the Slovenian network technology and security forum NOG (Network Operators Group).

E-Mail: In the field of e-mail security and protection against undesired or malignant messages we have continued in-house software development. The existing Bayes classification systems were expanded to use a Redis database instead of the existing RDBMS, which improved the classification performance and scalability considerably. The new approach has been included in the open source SpamAssassin package and will be available in the 3.4.0 release of the package. Based on this experience with Redis, we have modified the Amavis e-mail filtering system to automatically store received-message source IP addresses with assigned measures in a Redis database so that



Cryptography and certification: Currently, DNSSEC signed internet domains are the exception rather than the rule in Slovenia, and the ijs.si domain is not yet signed. However, both DNS servers at the institute have been performing the cryptographic verification procedure since the beginning of 2013. The signing of our domains has been postponed intentionally



Figure 2: GÉANT Infinera network provides higher capacities and dedicated links (Ljubljana bottom right)

since the technology incurs a built-in danger of major denial of service in the case of an error or technical mistake. In order to ensure correctness, a gradual approach to implementation has been adopted. In the first stage, we introduced two different automated mechanisms for the verification of signatures and procedures that have been tested extensively. Based on this security layer, we plan to officially start signing our domain with DNSSEC in 2014. Later, we will introduced the DANE system (integration of TLS certificates with the DNS system) in e-mail transfers and publishing SSHFP records via DNS servers. In addition, we have improved our existing certification support based on the SiGNET CA scientific certificate PKI system by introducing free COMODO server certificates, courtesy of Arnes support, since COMODO certificates are recognised by all the major operating systems and browsers.

We have encouraged the wider adoption of our existing VPN infrastructure, intended to enable our users in remote locations to connect to the institute network securely. The use has risen considerably among the travelling users and conference visitors who often have to deal with networks that block certain types of connections. The VPN is quite resilient and capable of transferring data over a virtual https connection, circumventing such measures.

Network services. The NIC provisions, develops and maintains a number of core and additional ICT services. The most important among these are e-mail (e-mail routing and delivery, in-box management, direc-

tory management, web mail services etc.) and world wide web support (central web server, web hosting for users, departments and projects, web directory). Secondary services are provided in support of certain core or specific activities at the Institute, such as web presentations, a conference system, supervision and monitoring, etc. In some of these services the NIC is directly invested in the software or infrastructure development, such as the network time services and e-mail filtering and security, while others are simply administered and maintained.

In spite of limitations of space and energy, a number of upgraded and new network services mark increased support for research groups, internal and external collaboration, software development, data protection and the provisioning of infrastructure, services and licences.

The third NIC service category is comprised of services supporting our

users (calendaring, event management, directories) and software/system developers (code repositories, integration and verification, licence management). In addition, we provide physical server hosting and management, aimed primarily at larger projects and systems, the administration of directories for personal computing and user management (such as departmental single sign-on or directory services) and the administration of mission-critical workstations and components.

In 2013 we continued the reorganisation effort started in 2011 with the goal of improving our systems automation and provisioning to manage the increasing load on our personnel due to higher demands and the rise in user numbers, network traffic and supported services. Our efforts stalled in 2013 due to the physical limitations of our computing centre room, its electrical and cooling systems. We have upgraded the electrical installations to partially permit further additions to installed equipment but have not been able to procure an upgrade to the existing cooling system, which has proven inadequate in the last three summers. This has prompted the partial downsizing (discontinuation of non-critical service in hot months) and postponing of a number of larger projects (new archival systems, off-site backup system arrangement with Reactor Infrastructure Centre Podgorica, on-demand physical and virtual servers and data servers for temporary data storage) to 2014.

A number of core services have received hardware and software updates in 2013: in particular the central webmail relay server, web proxy, IMAP service (end user facing server, now with a larger data pool and bigger personal quotas), backup server for managed servers and the authoritative DNS server for our domain. The central web server has been completely replaced and the hosting server (where 45 sites were hosted at the end of



Figure 3: Upgraded electrical installation at the NIC computing centre allowed even denser equipment installation.

the year) has also received a major update. Since the load on our personnel has significantly increased due to the number of users and services, we have begun to implement automation for the maintenance and provisioning of certain core services which we will, physical conditions permitting, extend to on-demand services for users. We have implemented the Poudriere build system for pkg, Jenkins CI system and a testing deployment of the Salt and Puppet configuration/provisioning system.

Due to demands from research departments, we started managing central application development and store management for mobile and desktop software dissemination systems (such as Apple AppStore, Google Play, Blackberry World, Microsoft Store) so that software developers and their departments are free from management

burden and membership costs. In addition, we have started a software repository with development and continuous integration support (based on open-source packages Git, GitLabHQ, GitLabCI).

Due to increased interest in a number of services (Eduroam, VPN, web hosting, development tools, etc.) we improved and extended our web-based documentation.

Network computing. In the field of network computing technology and infrastructure, understood as a superset of high throughput computing, high performance computing, grids and clouds (ICT as a service), the NIC is collaborating with individual computing clusters at the institute and is also involved directly in the Slovenian

Our researchers can now use a single authentication mechanism and a single user API to access any of the computing clusters at the Jožef Stefan Institute, Slovenian SLING network computing collaboration or the European EGI infrastructure, putting tens of thousands of computing cores at your fingertips. National Grid Initiative SLING as a funding member and core partner. The NIC maintains the Slovenian certification agency SLING CA for science, research and grid computing and takes part in the maintenance and support of the core grid network services.

In 2013 we have been successful in continued operations of CiPKeBIP/ E8 cluster and the integration of existing JSI clusters in the SLING network running ARC (Nordugrid Advanced Resource Connector) grid middleware. The inclusion of the KRN cluster completed the process of integration. At this point, any institute researcher can use the same interface to access any of the

computing resources in the institute or Slovenian computing network, i.e. Arnes (currently 2300 cores), SiGNET (2194 – F9), Atos (1477 – F1), KRN (1176 – R4/F8) or CiPKeBIP/E8 (984). The same UI and SiGNET CA certificate allows all users in Slovenia to access any other grid-enabled resource in the world.

In the context of SLING, we initiated a cluster administrator working group with regular meetings that facilitates collaboration considerably. But since we were unable to provide acceptable room and infrastructure for our clusters, we were unable to assist with the expansion of the existing resources. Expansion remains of crucial



Figure 4: Network computing uses the advances in network development and computing power to present new computing models to the users in Slovenian SLING network and the European Grid Initiative.

importance, since it is a condition for further collaboration in a number of large international research projects and groups, many of which already count the Jožef Stefan Institute as a member.

In the domain of network computing we have been involved not just in SLING, but also in the European Grid Initiative EGI, NorduGrid ARC collaboration and a number of international projects (ATLAS – dedicated link, Belle2 – computing grid network support planning). SLING has supported a number or research projects and applications in 2013, including high-energy physics, medical sensor and image analysis, theoretical physics, astrophysics, biochemistry, protein folding simulation, knowledge technologies, statistical analysis and fluid dynamics. 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.

R&D GRANTS AND CONTRACTS

 Slovenian Literature in Unknown Early Modern Manuscripts: Information-Technology Aided Analyses and Scholarly Editions Jan Jona Javoršek, B. Sc.

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- 5. Matjaž Levstek
- 6. Mark Martinec, B. Sc.
- Janez Srakar
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SCIENCE INFORMATION CENTRE

SIC

The Jožef Stefan Institute Science Information Centre is the central Slovenian physics library and one of the largest special libraries in Slovenia. Our main tasks are the acquisition, archiving, and loan of books and periodicals, and the input, update and control of bibliographic data of the Institute staff, as requested by the funding ministry.

Our collection covers the fields of physics, chemistry, biochemistry, electronics, information science, artificial intelligence, nuclear technology, energy management and environmental science. We are a full member of the Slovenian library cooperative, COBISS, and use their services to catalogue and loan our materials. You can check what is new in the library, browse our online catalogue, or send inter-library loan requests using our WWW site.

We supplement our comprehensive print collection of core journals with the electronic editions, offered through our WWW site. We subscribe to the electronic collections offered by ScienceDirect, Springer Link, IEEExplore, Stanford HighWire Press, ACS online editions, AIP electronic editions, IoP online journals, Wiley Interscience. We provide access to the SCOPUS, INSPEC, Crossfire Beilstein, and Web of Science databases, and the Dialog on-line database services.

 Head:

Dr. Luka Šušteršič

We manage a bibliographic database of the Institute's production. The database contains about 80,000 records, going back to the Institute's inception in 1949. The records of last year's work are included as part of this report.

STAFF

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- 1. Dr. Luka Šušteršič, Head
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- Jože Škulj
- Branka Štrancar
- 9. Nada Tratnik
- 10. Saša Žnidar

ENERGY EFFICIENCY CENTRE

EEC

The basic activities of the Energy Efficiency Centre are in the efficient use of energy, long-term planning in energy and the reduction of greenhouse-gases emissions. The centre is a focal point for the collection and transfer of energy-efficiency technologies to energy users, the state, energy service and equipment providers, and other interested agencies. At the same time it covers the environmental effects of energy use and conversion. The most significant part of the EEC's activities is thus cooperation with state institutions in the preparation of strategic documents and legislation in the field of efficient energy use, energy planning, distributed electricity production, emissions trading; nevertheless it still remains strongly connected, by its consulting and training role in energy, with industrial companies and other institutions as well as being more and more involved in European research projects.



Energy and the environment

In 2013 the Energy Efficiency Centre with its professional work ensured high-quality support to ministries in Head: the preparation of development strategic documents and the transfer of EU legislation in the field of energy planning, energy efficiency, use of renewables and greenhouse-gases emissions and the reduction of other pollutants. The accepted EU climate-energy package set new and ambitious goals for Slovenia regarding the increase

of energy efficiency, the exploitation of renewables and the reduction of greenhouse-gases emissions. Efficient energy use is a priority field for achieving these goals, in accordance with the requirements of the European Commission and a new directive on energy efficiency (2012/27/EU). Strategic studies for setting national energy goals till 2030 and updated energy balances of the RS until 2030 were elaborated for the Ministry of Transport and Infrastructure. The EEC carried out an evaluation of the operation of the support scheme for the production of electricity from renewable energy sources and cogeneration, together with proposals for upgrading and support tools for planning scheme operation.

The center cooperates with the Statistical Office of the Republic of Slovenia, where it prepares a model calculation of fuels and energy use in

households for the national energy statistics. In 2013 the center continued with activities of the state referential centre for energy by the preparation of a set of indicators for energy and environment, as well cooperating in the carrying out of the research of energy efficiency REUS in households and services.

In the field of the reduction of greenhouse-gases emissions, the center elaborated for the Ministry of Agriculture and Environment strategic studies for the preparation of the Operational programme of GHG emissions reduction in the period 2013–2020 with an analysis of the potentials for emissions reduction until 2030 and offered professional support when discussing pollutants from the NEC directive.

A target research project Environment print of agriculture and food processing industry, which by carrying out of support tools established a completely new environment for the environment and energy evaluation of activities and quality support for contractors in the transition to sustainable production, was concluded very successfully and resoundingly.

Promotion of efficient energy use and energy consulting

In 2013 the Energy Efficiency Centre continued with its training activities where the sixth cycle of energy managers' training was successfully concluded within the European programme EUREM. In the autumn already the seventh cycle of training started. Due to the very positive reaction of participants and their interest (in Slovenia there is already more than 140 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.





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 2: Main award in the category of large enterprises 2013 at the 4th Conference of European energy managers in Nuremberg to Mr. Aljaž Bratina for the project Strategies of energy efficiency of Pošta Slovenije (mentor M.Sc. Boris Sučić, EEC)



Figure 3: Optimization of the operation of ship-to-shore cranes in Luka Koper



Figure 4: Training "Public orders and energy efficiency in buildings" in the framework of the project EFFECT.

In 2013 the Center of Energy Efficiency carried out several consulting tasks in industry and the public sector, where in particular the cooperation with Luka Koper was strengthened. Great economic effects with a reduction of energy-use costs were achieved by the execution of deepened energy audits of individual terminals and by an analysis of the possibilities for the introduction of advanced technologies for transloading. The professional cooperation with Salonit Anhovo, Termoelektrarna toplarna Ljubljana, BTC, General Hospital Brežice, Klinika Golnik, etc., has been continued.

The center continued its professional cooperation with the company Petrol d.d. in carrying out the largest programme of large consumers for ensuring energy savings of end users and expanded its activities also to the company GEN-i. d.o.o.

The center prepared the programme for the jubilee fifteenth conference "Energy Managers Days", the annual meeting of energy managers, with more than 200 participants, which confirms the quality and public profile of the EEC professional work.

International cooperation

The center cooperated in the preparation of the project and investment documentation for the integrated energy renovation of buildings at the Reactor Centre JSI in Podgorica, where the JSI acquired, from a tender of the Ministry for Education, Science, Culture and Sport, \in 1,6m of grants for carrying out renovation, which should start in 2014.

In 2013 the EEC carried out as many as 15 international projects, financed from the European Union resources in the framework of the 7th Framework Programme and European Commission programme "Intelligent Energy for Europe" as well as MEDITERAN and South East Europe.

Projects cover activities in the fields of:

- development of innovative systems of energy use monitoring and management in industry (Life Saver, 7th FP),
- increase of energy efficiency of existing non-residential buildings with the introduction of the cost-effective optimization of energy systems Re-Commissioning (Re-Co),
- analysis of the impacts of the introduction of smart energy measurements on the use and costs of energy in low-income housing (Elih-MED),
- inclusion of criteria of energy efficiency in the public tenders (EFFECT),
- increase of transparency of markets with energy services (Transparense),
- compiling and elaboration of current data on renewable energy sources use (EurObserv`ER Barometer),
- monitoring and promotion of cogeneration development (CODE2),
- carryng out the EU directive on energy efficiency (CA EED),
- carryng out the EU directive on renewable energy sources (CA RES),
- monitoring of indicators for energy use and energy efficiency in the EU (ODYSSEE MURE EU-27),
- development and carrying out of integrated energy concepts in technological centres (Go ECO),
- central environment energy management as a tool for survival (CEEM),
- advanced financial platform for the promotion of green growth and eco-innovations (Ecofunding),
- strengthening of policies of urban sustainability (UrbanEmpathy).

The projects include cooperation with research and development organisations from Europe with a strong emphasis on concrete applications and the promotion of energy efficiency. In the framework of each project EEC staff took part in numerous foreign professional meetings and visits.

Some outstanding achievements in the past year

- 1. Preparation of several key support documents for the government of the Republic of Slovenia in the field of energy policy (Green paper and strategic studies for the National Energy Programme), energy efficiency (First and Second National Action Plan for Energy Efficiency), renewable energy sources (Action Plan for Renewable energy sources for the period 2010–2020) and climate policy (Operative programme of GHG emissions reduction up to 2020).
- Establishment of energy managers training in the framework of the European project EUREM and professional support to industry and other institutions by carrying out energy audits, feasibility studies and other consulting (Goodyear, TE-TOL, Luka Koper, Salonit Anhovo, Telekom Slovenije, BTC, ELENA – Ljubljana, etc.).
- 3. Cooperation in different international projects in the framework of European Commission programmes in the fields of energy efficiency, energy management, combined production of electricity and heat, promotion of energy-efficient technologies and energy services, exploitation of wood biomass and others.

Organization of conferences, congresses and meetings

- 1. Energy Managers Days 2013 15th Meeting of energy managers of Slovenia, Portorož, Slovenia, 16.-17.4. 2013
- 2. With small steps to greater comfort and energy savings, Brežice, Slovenia, 23. 5. 2013
- 3. Energy efficient public procurement lighting, household appliances, computer equipment, Ljubljana, Slovenia, 6. 6. 2013
- 4. Training European energy manager, Ljubljana, Slovenia, 15.–18. 1., 20.–22. 3., 31. 5., 13.–14. 6. 2013
- 5. Public procurement and energy efficiency of buildings, Ljubljana, Slovenia, 27. 11. 2013
- 6. Roadmapping of cogeneration in Slovenia, Ljubljana, Slovenia, 26. 11. 2013
- Roadmapping of cogeneration in Poland, Warsaw, Poland, 4. 12. 2013

INTERNATIONAL PROJECTS

- 1. 7FP LifeSaver; Context Sensitive Monitoring of Energy Consumption to Support Energy Savings and Emission Trading in Industry European Commission
- Boris Sučić, M. Sc.
- IEE EurObservER2020; The EurObservER Barometer Backs the New RES Directive European Commission Dr. Fouad Al-Mansour
- ELIH-Med Energy Efficiency in Low-Income Housing in the Mediterranean Joint Technical Secretariat Med Programme
- Aleš Podgornik, M. Sc.EFFECT Upgrading of Energy Efficient Public Procurement for a Balanced Economic growth of SEE Area
 - Agenzia Regionale Per L'Energia Polona Lah. B. Sc.
- Re-Co; Re-Commissioning-Raising Energy Performance in Existing Non-Residential Buildings
 - European Commission
 - Barbara Petelin Visočnik, M. Sc.
- 6. EIE C.O.D.E. 2; Cogeneration Observatory and Dissemination Europe 2; IEE/11/910/ SI2.615940
 - European Commission
- Stane Merše, M. Sc. CEEM - Central Environmental and Energy Management as a Kit for Survival
- City Of Vienna, Department For EU-strategy
- Matevž Pušnik, M. Sc. 8. Go ECO; Development and Implementation of Integrated Energy Concepts in Business
- Parks European Commission
- Peter Bevk, B. Sc.
- 9. EIE pr. TRANSPARENSE; Increasing Transparency of Energy Services Markets European Commission
- Damir Staničić, M. Sc. 10. EIE - ODYSSEE MURE 2012; Monitoring of Energy Efficiency in the EU European Commission
- Dr. Fouad Al-Mansour 11. IEE; EurObservER, The EurObservER Barometer (2013-2016) European Commission

Matjaž Česen, B. Sc.

- MED EMILIE; Enhancing Mediterranean Initiatives Leading SMEs to Innovation in Building Energy Efficiency Technologies Joint Technical Secretariat Med Programme
 - Stane Merše, M. Sc.
- 13. MED pr.; ECOFUNDING; Innovative Funding Scheme for Energy and Eco Innovation Projects
- Joint Technical Secretariat Med Programme Polona Lah, B. Sc.
- URBAN EMPATHY Empowering Policies on Urban Sustainability Joint Technical Secretariat Med Programme Aleš Podgornik, M. Sc.
- SEE-ERA.NET PLUS ISEMIC Intelligent Information System for Monitoring and Verification of Energy Management in Cities University Of Zagreb Boris Sučić, M. Sc.

RESEARCH PROGRAM

 Modelling and Environmental Impact Assessment of Processes and Energy Technologies Dr. Fouad Al-mansour

R&D GRANTS AND CONTRACTS

- Environmental Footprint of Agriculture and Food Processing Industry and Technological Measures for its Lowering in the Future Dr. Fouad Al-mansour
- EIE- EUREM.NET, Training and Network of European Energy Managers, N 112/06; EUREM I-VII
- Boris Sučić, M. Sc.
 Evaluation of the Flywheel Technology in the Process of Energy Eecovery and Storage in a Mobile Gantry Crane - Case Study Port of Koper Port of Koper Boris Sučić, M. Sc.



NEW CONTRACTS

- 1. Strategic study for the Operation programme for greenhouse gasses reduction measures for the period 2013-2020 with an analysis of potential reduction by 2030 Ministry of Agriculture and the Environment Andreja Urbančič, M. Sc.
- 2. Development Project for Establishing a Platform of Advanced Services for Energy Management of Household Consumers Solvera Lvnx, d. d.

Aleš Podgornik, M. Sc.

- 3. Elaboration of a Concept and Methodology of the Research of Energy Efficiency of Slovenia for the Public and Services Sector Informa Echo, d. o. o.
 - Stane Merše, M. Sc.
- 4. Updating of energy balances and strategic studies for the determination of national energy goals Ministry of Infrastructure and Spatial Planning

Andreja Urbančič, M. Sc.

VISITORS FROM ABROAD

- Sara van Rompaey, European Commission, Brussels, Belgium, 17.-19. 9. 2013
- Prof. Eduardo Maldonado, University of Porto, Portugal, 17.-19. 9. 2013 2.
- 3. Dr. Christos Maxoulis, Scientific and technical chamber, Cyprus, 17.-19. 9. 2013
- Carles Sala, Generality of Catalonia, Barcelona, Spain, 17.-19. 9. 2013

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- Postgraduate

Matevž Pušnik, M. Sc.

Technical officers

Peter Bevk, B. Sc.

- Elaboration of a Strategic Study and a Model for the Design of Determination of Technologies Having Priority at Entering into the Support Scheme in Case of Limited Resources Ministry of Infrastructure and Spatial Planning
 - Stane Merše, M. Sc.
- 6 National Reference Centre for Energy and Refreshment of Energy and Environment Indicators 2013/14

Slovenian Environment Agency Matjaž Česen, B. Sc.

- Energy Consumption of Slovenian Households Based on Model Calculation for 2012 Statistical Office of the Republic of Slovenia Matjaž Česen, B. Sc.
- EU project GreenBerth Design of the Methodology for the Validation and Transfer of Technologies Relevant for Energy Efficiency Improvements in Ports' Operations Port of Koper Boris Sučić, M. Sc.
- Slobodan Sofeski, Chamber of small enterprises, Skopje, Macedonia, 9. 10. 2013
- 6. Stojan Dukoski, Company Key to the Hand, Skopje, Macedonia, 9. 10. 2013
- Nikola Nestoroski, Company Proaqua, Skopje, Macedonia, 9. 10. 2013
- 7. Matiaž Česen, B. Sc. 8
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- 14. Igor Ribič

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- Polona Lah, Andreja Urbančič, Barbara Petelin-Visočnik, Matjaž Česen, "Analiza delovanja podporne sheme in ocena njenega prispevka k doseganju nacionalnih ciljev na področju OVE in SPTE", In: Enajsta konferenca slovenskih elektroenergetikov, Laško, 27.-29. maj 2013, [Ljubljana, Slovensko društvo elektroenergetikov CIGRÉ - CIRED], 2013, 9 pp.

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14. Tomaž Vuk, Magda Gabrijelčič, Tomaž Fatur, Boris Sučić, "Kompleksno vrednotenje energetskih in okoljskih vidikov v energetsko intenzivni industriji - pristop LifeSaver na primeru podjetja Salonit", In: *15 let na poti energetske odličnosti: zbornik*, Barbara Petelin-Visočnik, ed., Stane Merše, ed., Ljubljana, Časnik Finance, 2013, pp. 137-142.

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- 1. Polona Lah, "Učinkovita raba energije in zelena javna naročila", In: *URE, energetika in okolje*, (Zbirka Zelena Slovenija), Jože Volfand, ed., Celje, Fit media, 2013, pp. 110-114.
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CENTRE FOR ELECTRON MICROSCOPY

CEM

The Centre for Electron Microscopy (CEM) has the function of a supporting infrastructure center at the JSI that comprises the equipment for electron microscopy that is necessary for the research work of the departments K5, K6, K7, K8 and K9. Other JSI departments, research institutes, universities and industry also have access to the equipment. The users of the CEM equipment are researchers in the field of materials science that are involved in the chemical and structural analysis of materials on the micro and atomic scales. The major equipment of the CEM represents two scanning electron microscopes (JSM-840A and JSM-5800) and two transmission electron microscopes (JEM-2000FX and JEM-2010F). The CEM coworkers also manage the transmission electron microscope JEM-2100 that belongs to the Center of Excellence NiN and in 2009 a newly installed field-emission scanning electron microscope JSM-7600F that was a joint purchase by ten JSI departments and also the faculties NTF and FKKT of the University Ljubljana. In 2010 the electron microscopes were upgraded with the following analytical attachments that were purchased by the Centre of Excellence NAMASTE: CCD camera on JEM-2010F, ADF detector on JEM-2010F and EBSD system on JSM-7600F.



Prof. Miran Čeh

Scanning electron microscopy (SEM) is used for the morphological studies of either fractured or polished surfaces. Since both scanning electron microscopes are equipped with X-ray spectroscopy (EDXS, WDXS), qualitative and quantitative chemical analyses on the microscale is also possible. Since only a few μ m³ of the material is nondestructively analyzed, the term electron-probe microanalysis (EPMA) is used for such analytical work. Apart from EDXS and WDXS, the new FEG-SEM JSM-7600F is also equipped with electron lithography.

When the structural features on the nanoscale are investigated, however, various techniques for transmission electron microscopy (TEM) are used. In particular, the JEM-2010F is a state-of-the-art TEM/STEM microscope with a FEG (field-emission gun) electron source with a point-to-point resolution below 0.19 nm, which is more then sufficient to observe the atomic columns in crystalline materials. JEM-2010F is also equipped with an annular dark-field detector (HAADF-STEM) for so-called Z-contrast imaging, which enables chemical analysis of a single atomic column on the basis of the measured intensities. Both transmission electron microscopes are additionally equipped with analytical systems for chemical analysis (EDS, EELS). The CEM also comprises the equipment for

SEM and TEM specimen preparation, which is the first starting step for all electron microscopy observation procedures. Especially important are the high- and low-energy ion-millers, which enable the preparation of thin foils that are transparent to high-energy electrons.

The analytical work that is performed on the CEM equipment varies, concerning both the investigated materials and/or the applied electron microscopy techniques. While scanning electron microscopy is used mainly for microstructural characterization and the chemical analysis of polycrystalline ceramic materials (functional ceramics, engineering ceramics, bio-ceramics, and composites), magnetic materials, glasses, metals, alloys, etc., transmission electron microscopy is used for structural and chemical investigations of grain boundaries, planar faults, dislocations and precipitates within the same materials. The structural and chemical analysis of grain boundaries is especially important since it is known that the final physical properties, to a large extent, depend on the structure and chemistry of grain boundaries.

In order to be able to perform electron microscopy investigations it is imperative that the equipment in the CEM is well maintained. In view of this, one of the main tasks is to achieve the maximum possible operational time of the microscopes. This complex and expensive equipment needs regular daily maintenance, apart from servicing. Other activities of the CEM are the organization of training courses for the operators and the implementation of new analytical methods, which is realized with the help of the CEM co-workers.



Figure 1: HR-TEM image of milled Nb₂O₅ particles with insets showing FFTs of the selected areas. Nanocrystals of tens of nm are clearly seen on the surface of the larger particle. The diffraction spots of these nanocrystals obtained with a fast Fourier transform (FFT) (inset left) correspond to the orthorhombic (001) plane reflections, while the spots from the larger particle (inset right) correspond to the monoclinic (-101) plane reflections.

Electronic Ceramics: A. Benčan (J. Hreščak, A. Benčan, T. Rojac, B. Malič, J. Eur. Ceram. Soc., 2013, 33 [15-16], 3065-3075)



Figure 2: Surface of bioactive calcium phosphate coating. Engineering Ceramics: M. Štefanič



Figure 4: Scanning electron microscopy (SEM) image of $BaFe_{12}O_{19}$ nanoplatelets textured in a magnetic field. Synthesis of Materials: D. Lisjak



Figure 3a: HRTEM image contact (130) twin boundary in chrysoberyl from the Pratinhas locality in Bahia (Brazil). Transmission electron microscopy (TEM; JEM-2100, Jeol, Japan) using high-resolution TEM and electron-diffraction techniques were used to study the crystallography of the twin boundary. The crystal was oriented along the [001] orientation. The twin boundary is characterized by a straight line. Electron diffraction patterns recorded on both sides of the boundary show that the two crystal domains are related by a 180° rotation around the crystallographic [110]axis with (130) plane as the twin interface.

Figures 3b,c. HRTEM image of thin TiO_2 precipitates in chrysoberyl crystal. Precipitates lie parallel to the two equivalent {120} planes of chrysoberyl, which intersect at an angle of 98.7°. Some precipitates are composed of only simple slabs of rutile, but quite often L-shaped rutile precipitates are observed. They are composed of two rutile crystals coinciding at the L-junction with their c-axes enclosing an angle of 7.5°.

Nanostructured Materials: S. Drev



Figure 5: Hydrothermally synthesized BaTiO₃. Advanced Materials: M. Maček

STAFF

Researchers 1. Prof. Miran Čeh, Head Technical and administrative staff 2. Hamdija Hodžić, B. Sc.

CENTRE FOR KNOWLEDGE TRANSFER **IN INFORMATION TECHNOLOGIES CT-3**

The Centre for Knowledge Transfer in Information Technologies performs educational, promotional and infrastructural activities and provides for the direct exchange of information and experience between researchers and the users of their research results.

By partnering and actively engaging in different European research projects the centre successfully extends its activities to research and development. Most of the research is performed in the area of knowledge management for traditional and emerging forms of organizations, like networked and virtual organizations. In 2013 the centre was active in several European projects from FP7: PASCAL2 (Pattern Analysis, Statistical Modelling and Computational Learning 2), METANET (Multilingual Europe: a Technology Alliance), RENDER (Reflecting Knowledge Diversity), ALERT (Active support and Real-time Coordination based on Event Processing in Open Source Software Development), PLANETDATA (A European Network of Excellence on Large-Scale Data Management), e-LICO (An e-Laboratory for Interdisciplinary Collaborative Research in Data Mining and Data-Intensive Science), TRANSLECTURES (Transcription and Translation of Video Lectures), X-LIKE (Croslingual Knowledge Extraction), Head: MOBIS (Personalized Mobility Service for energy Efficiency and Security through Advanced), MEDIAMIXER (Com- Mitja Jermol, M. Sc. munity Set-up and Networking for the Remixing of Online Media Fragments), NRG4CAST (Energy Forecasting), SOPHOCLES (Self-Organised information Processing, Criticality and Emergence in multile), CENTRAL COMMU-



NITY (Emerging communities for collective innovation in Central Europe), SYMPHONY (Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy), X-LIME (crossLingual crossMedia knowledge extraction), PROASENSE (The Proactive Sensing Enterprise).

In 2013 the Centre for Knowledge Transfer in IT

In 2013 the centre was active in 16 European projects. The centre prepares and organizes carefully designed educational events, such as conferences, seminars, workshops, and summer schools. They are targeted at experts

who would like to apply the latest knowledge and achievements from intelligent data analysis, knowledge technologies, data mining, text mining and decision support to the areas of network organizations, business decisions, finance, marketing, automatization and process control. A special consideration is put on the managers and decision makers who are aware of the strengths and benefits to the success of their business.

All educational events are designed to transfer basic, additional and the latest expert knowledge to the companies, research and educational organizations. In order to make the knowledge transfer efficient we are combining traditional and ICT-supported training methods. For this purpose we are operating a number of training web portals. The most popular one is http:// videolectures.net/. It now offers more than 18,021 recorded tutorials from different scientific events and is visited monthly by an average of 146,000 visitors from around the world. The main purpose of the portal is to provide free and open access to high-quality video lectures presented by distinguished Figure 1: Award ceremony where the Videolectures. Net portal was selected scholars and scientists at the most important and prominent events. In today's world VideoLectures.NET presents a free knowledge hub, a way of

opening up education to everyone for everyone as there is a great need to share educational content on all levels in order to benefit society and foster the economy. It also gives a learning opportunity to audiences of all social levels.

We have successfully collaborated within the Videolectures.net portal with some of the top ten American Universities MIT (Massachusetts Institute of Technology), University of California - Berkeley, YALE, John Hopkins University, University of California, Irvine, and Carnegie Ethics Studio, as well as with the European CERN and ETH from Zurich. VideoLectures.Net has CT3 is operating the web portal http://

strong connections in OpenCast Foundation, OpenCourseWare Consortium and Knowledge 4 All Foundation Ltd.

The centre also operates a web portal http://www.ist-world.org that offers services for automatic data collection and an analysis of European

was actively involved in 16 European projects.



as the WSIS+10 Global Champion

videolectures.net/, which is now the largest world reference portal presenting high-quality scientific lectures.



Figure 2: The creators and authors of the Videolectures.Net portal

In 2013 the portal won the World Summit Award for the best product in the field of creative and innovative e-content in the past decade, granted by the United Nations and UNESCO. research. The user can perform several simple and complex analyses, predictions and detect trends in research. The database currently contains about 100,000 research organizations, 42,500 research projects and around 2 million experts from Europe. This is an exceptional web service that is being visited daily by an average of 6,000 unique visitors.

We organized the 8th Student Competition in Computer Science, attended by 133 students from Slovenian secondary schools. We have also organized project meetings for different EU projects (RENDER, PLANET DATA, MOBIS and X-LIKE) and an international workshop for the EU project TRANSLEC-TURES, MediaMixer and X-like "Internet of Education", which was attended by 99 experts. In collaboration with the Slovenian Chamber of Commerce we organized a "Regional ICT RTD Foresight Open Consultation". There were 67 experts from Slovenia and abroad from the e-Health, e-Government and e-Content area.

With our strategic partners we organized the "First Center for Knowledge transfer workshop" with the aim of establishing a new business vision and strategy for the Videolectures.Net portal. In collaboration with the Commission for the Prevention of Corruption we organized a technical workshop "Use of advance information technology", attended by 60 experts.

In 2013 we started negotiations about new initiative "Opening Up Slovenia". The OpeningUpSlovenia case study framework will foster research, development, education and other relevant activities through national and

EU programmes (i.e., Erasmus+ and Horizon 2020) related to all aspects of open education, by allowing the rigorous, transparent, and replicable testing of open learning environments, open education theories, new business models, organisational forms, open education software, as well as new and emerging technologies in the education technology market. This unique experimental platform will be sufficiently large, open and flexible to provide for horizontal and vertical links within the education system involving education, research and business institutions, as well as institutions from the European Union, to stimulate the development of new open education frameworks

by targeting different groups and including experimental advanced research and users' realistic assessment.

Our role in the FP7 integrated projects XLike "Cross-lingual Knowledge Extraction" and RENDER – Reflecting Knowledge Diversity, and in three networks of excellence, PASCAL2, PLANETDATA and META-NET, was the support and coordination of all educational and dissemination activities as well as knowledge transfer.

Awards and appointments

In 2013 we began the initiative

solutions for "open education".

"OpeningUpSlovenia", which will create an

international partners will develop and test their

environment in which the Slovenian and

1. United Nations and UNESCO award Videolectures.Net portal for best educational product of the decade. The VideoLectures.Net was selected as the winner in the "e- Science & Technology" category.

Organization of conferences, congresses and meetings

- Regional conference "SEE Regional Open Consultation for foresight in ICT Research, Development and Innovation", Ljubljana, 21. 1. 2013
- 2. Project meeting of the EU project RENDER, 4.–5. 2. 2013
- 3. Project meeting of the EU project PLANET DATA, 7.–8. 2. 2013
- 4. Kick-off meeting of the EU project MEDIAMIXER, 14.–15. 2. 2013
- 5. 8th Student competition in computer science, Ljubljana, 23. 3. 2013
- 6. Project meeting of the EU project MOBIS, Ljubljana, 15.-16. 10. 2013
- Technical workshop "Use of advance information technology: the anti-corruption body's perspective", Ljubljana, 28.–29. 10. 2013
- 8. Organization of the international conference "Internet of education" Ljubljana, 11.-12. 11. 2013

INTERNATIONAL PROJECTS

- Video recording and post production of the lectures Foreign Buyers Mitja Jermol, M. Sc.
- 7FP PASCAL2; Pattern Analysis, Statistical Modelling and Computational Learning 2 European Commission Mitja Jermol, M. Sc.
- 7FP MetaNET; Technologies for the Multilingual European Information Society European Commission Mitja Jermol, M. Sc.
- A. 7FP RENDER; Reflecting Knowledge Diversity European Commission
 Mitia Jermol M. Sc.
- Mitja Jermol, M. Sc. 5. 7FP - PlanetData European Commission
- Mitja Jermol, M. Sc. 6. 7FP - ALERT; Active Support and Real-time Coordination based on Event Processing in Open Source Software Development
- European Commission Mitja Jermol, M. Sc.
- 7FP transLectures; Transcription and Translation of Video Lectures European Commission Mitja Jermol, M. Sc.
- 7FP Sopholes; Self-Organised information PrOcessing, CriticaLity and Emergence in multilevel Systems
- European Commission Marjana Plukavec, B. Sc.
- 7FP² MEDIAMIXER; Community Set-up and Networking for the Remixing of Online Media Fragments European Commission Mitja Jermol, M. Sc.

VISITORS FROM ABROAD

- 1. Yannis Tolias, Innovatia Systems, Greece, 22. 1. 2013
- 2. Lyndon Nixon, STI International, Austria, 9. 9. 2013

- 10. 7FP MobiS: Personalized Mobility Services for Energy Efficiency and Security through Advanced Artificial Intelligence Techniques European Commission
- Mitja Jermol, M. Sc. 11. 7FP - ProaSense; The Proactive Sensing Enterprise European Commission Mitja Jermol, M. Sc.
- 7FP SYMPHONY; Orchestrating Information Technologies and Global Systems Science for Policy Design and Regulation of a Resilient and Sustainable Global Economy European Commission
- Mitja Jermol, M. Sc. 13. 7FP - xLiMe; CrossLingual CrossMedia Knowledge Extraction European Commission
- Mitja Jermol, M. Sc. 14. 7FP - X-Like; Cross-lingual Knowledge Extraction European Commission
- Mitja Jermol, M. Sc. 15. 7FP - NRG4CAST; Energy Forecasting European Commission Mitja Jermol, M. Sc.
- CE Central Community-Emerging Communities for Collective Innovation in Central Europe City of Vienna, Department for EU-strategy

Mitja Jermol, M. Sc.

R&D GRANTS AND CONTRACTS

- 1. Cloud Assisted Services: CC CLASS Mitja Jermol, M. Sc.
- 3. Raphael Troncy, Eurecom, France, 2. 10. 2013
- 4. Vasileios Mezaris, CERTH-Centre for Research & Technology, Greece, 14. 11. 2013

STAFF

Technical officers

- 1. Mitja Jermol, M. Sc., Head
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- 3. Marjana Plukavec*, B. Sc.
- 4. Špela Sitar, B. Sc. **Technical and administrative staff**
- 5. Gaber Cerle, B. Sc.

- 6. Mihajela Črnko
- 7. Ana Fabjan
- 8. Adis Krečo, B. Sc.
- 9. Monika Kropej, B. Sc. 10. Tanja Zdolšek, B. Sc.

Note:

* part-time JSI member

MILAN ČOPIČ NUCLEAR TRAINING CENTRE ICJT

The mission of our training centre is training in the field of nuclear technologies and radiation protection. In addition, we are actively informing the public about these technologies.

Training in the area of nuclear technologies is our primary mission. The course *Nuclear technology*, which is the initial theoretical training of future control-room operators, ended in the spring of 2013. This was probably the end of 5-year-long intensive training of new staff for NPP Krško, where a change of generations took place. In the future we expect to conduct the Nuclear Technology course every second year. There was also a course *Basics of nuclear technology*, which is intended for the non-control-room personnel of NPP and participants from other organizations.

There were 25 radiological protection training courses for the medical, industrial and research use of radioactive sources. Two courses were intended for the security personnel of Reactor Centre Brinje and for the transport of nuclear materials.

We have conducted two international courses, funded by EU through the ITER consortium. The bulk of lectures Head: were given by experts from the Reactor Engineering Division (R-4) and from the Reactor Physics Division (F-8). **Prof** Public information remains a very important part of our activities. Groups of visitors (mainly schoolchildren,

students and various societies) were regularly attending the lectures on electricity from nuclear energy, on radioactive waste, and about fusion. They have also visited the permanent exhibition on nuclear energy. Altogether, there were 161 groups or 7063 visitors this year. Since 1993 our information centre was visited by a total of 149,743 pupils, teachers and other visitors. A significant contribution to public information is the enlarged and revised second edition of the Mini Encyclopaedia of Nuclear Energy that we pub-

We have prepared a thoroughly revised and expanded second edition of the bilingual publication "Mini Encyclopaedia of Nuclear Energy".

lished in July. This bilingual publication is distributed free of charge to our visitors. We have continued monitoring and analysing media reports on nuclear energy. An important part of the information activity is the *Fusion Expo* project, which is funded by the European Fusion Development Agreement. The travelling exhibition on fusion has been set up in London (United Kingdom), Goteborg (Sweden), Tartu (Estonia), Rust (Germany), Prague (Czech Republic) and Antwerp (Belgium).



Figure 1: Conclusion of the Nuclear Power Plant technology course



Figure 2: Exercise of trainees in the control room of the TRIGA research reactor



Prof. Igor Jenčič

Table of training activities at Nuclear Training Centre in 2013					
Date	Title of the course	Partici- pants	Lecturers	Weeks	Participants × weeks
5. 11. 12-5. 4.	Nuclear technology. Theory	23	19	13	299
28. 14. 2.	Radiation protection for RP department staff - Refresher course	9	4	1.0	9.0
11. 2.	Radiation protection for workers at Ljubljana Airport	7	1	0.2	1.4
18. 222. 2.	Radiation protection RZ2 for NPP subcontractors	22	7	1.0	22.0
25. 227. 2.	Radiation protection for industrial and other practices (unsealed sources)	2	5	0.6	1.2
25. 227. 2.	Radiation protection for industrial and other practices (sealed sources)	8	4	0.6	4.8
5.3.	Radiation protection for industrial and other practices (unsealed sources) - Refresher course	2	5	0.2	0.4
5. 36. 3.	Radiation protection for industrial and other practices (radiography) - Refresher course	2	4	0.4	0.8
5.3.	Radiation protection for industrial and other practices (sealed sources) - Refresher course	26	4	0.2	5.2
5.3.	Radiation protection for industrial and other practices (measurement of roadway density and humidity) - Refresher course	4	4	0.2	0.8
7. 3.	Training extension for RP Officers	8	2	0.2	1.6
6. 54. 6.	Basics of nuclear technology. Theory	11	13	4.4	48.4
14. 515. 5.	Annual refresher course for security officers	13	8	0.4	5.2
20. 524. 5.	Training course on "Requirements and safety evaluation of PSA for NPP"	12	9	1.0	12.0
22.523. 5.	Security officers for transport of nuclear materials - Refresher course	13	7	0.4	5.2
5. 628. 6.	Basics of nuclear technology. Systems	12	11	3.4	40.8
4. 7.	Radiation protection for industrial and other practices (sealed sources) - Refresher course	2	1	0.2	0.4
2.96.9.	Training Course on "Safety evaluation of SAR and oversight for Research Reactors"	14	7	1.0	14.0
3. 9.	Radiation protection for industrial and other practices (sealed sources) - Refresher Course	3	1	0.2	0.6
7. 10.–9. 10.	Radiation protection for industrial and other practices (unsealed sources)	2	5	0.6	1.2
7. 10.–16. 10.	Radiation protection for Dental Radiography	2	5	0.4	0.8
7. 10.–18. 10.	Radiation protection for medical and veterinary workers - Nuclear medicine workers	6	10	1.0	6.0
7. 10.–10. 10.	Radiation protection for industrial and other practices (measurement of roadway density and humidity)	1	4	0.8	0.8
7. 10.–9. 10.	Radiation protection for industrial and other practices (sealed sources)	7	4	0.6	4.2
15. 1018. 10.	Radiation protection for Nuclear Medicine Dpt Refresher course	2	7	0.4	0.8
15. 1017. 10.	Radiation protection for industrial and other practices (radiography) - Refresher course	2	4	0.4	0.8
15. 10.	Radiation protection for industrial and other practices (measurement of roadway density and humidity) - Refresher course	2	4	0.2	0.4
15. 10.	Radiation protection for industrial and other practices (unsealed sources) - Refresher course	9	5	0.2	1.8
15. 10.	Radiation protection for industrial and other practices (sealed sources) - Refresher course	14	4	0.2	2.8
16. 10.	Radiation protection for dental radiography - Refresher course	0	1	0.2	0.0
17. 10.	Training extension for RP officers	7	2	0.2	1.4
25. 1127. 11.	Radiation protection for workers of Cinkarna Celje Company	4	1	0.4	1.6
TOTAL		251	172	34.2	495.4



Figure 3: Lecture about radioactivity for school children

INTERNATIONAL PROJECTS

- 7FP EAGLE; Enhancing Education, Training and Communication Processes for Informed Behaviors and Decision-making related to Ionizing Radiation Risks European Commission Rado Istenič, B. Sc.
- 7FP Fusion Expo; Fusion Expo Support Action under EFDA Work Programme, Task Agreement WP10-PIN-FUSEX Ministry of Education, Science and Sport
- Tomaž Skobe, B. Sc. 7FP - FURATOM: Public Information in the
- 7FP EURATOM; Public Information in the Association 6.1.1-FU Ministry of Education, Science and Sport Prof. Igor Jenčič
- Realization of the International Workshop: "Group Fellowship Training Programme on Research Reactors" (IAEERRI11, IAEERRI11A, IAEERRI12), ICJT, 7.-18.3.2011; 7.-18.11.2011, 1.-12.10.2012 IAEA - International Atomic Energy Agency Saša Bobič
- Training and Tutoring for Experts of the NRAs and their TSOs for Developing and Strengthening their Regulatory and Technical Capabilities - INSC Project MC.03/10 -LOT 1: Training and Tutoring for Nuclear Regulatory Authorities and their TSO's: ITER-consult Srl Saša Bobič
- Edition of Slovene-English Publication "Mini Encyclopaedia of Nuclear Energy" Foreign Clients Prof. Igor Jenčič
- Design, Development and Delivery of Training Material for the Train-the-Trainer's Package on Nuclear Safety IAEA - International Atomic Energy Agency Prof. Igor Jenčič

R&D GRANTS AND CONTRACTS

- 1. Trainings of the RZ for Foreign Market Matejka Južnik, M. Sc.
- 2. Services in the Year 2013 Matejka Južnik, M. Sc.



Figure 4: Lecture about energy for primary school children



Figure 5: Mini Encyclopaedia of Nuclear Energy

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- Rado Istenič, B. Sc.
 Matjaž Koželj, M. Sc.
- Matjaz Rozelj, M. Sc.
 Nataša Medved, B. Sc., left 01.09.13
- 6. Tomaž Skobe, B. Sc.
- 7. Vesna Slapar, B. Sc.
- 8. Luka Tavčar, B. Sc.
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- Technical and administrative staff
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 Matejka Južnik, M. Sc.
- 12. Borut Mavec, B. Sc.



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PUBLISHED CONFERENCE CONTRIBUTION

- Radko Istenič, Igor Jenčič, "Public Opinion about Nuclear Energy-Year 2013 Poll", In: *Proceedings*, 22nd International Conference Nuclear Energy for New Europe - NENE 2013, Bled, September 9-12, Leon Cizelj, ed., Matjaž Leskovar, ed., Mitja Uršič, ed., Ljubljana, Nuclear Society of Slovenia, 2013, 6 pp.
- Matjaž Koželj, "Where is the border between professional and radiation protection education and training", In: *ETRAP 2013*, 5th International Conference on Education and Training in Radiological Protection, 12-

15 March, Vienna, Austria, Brussels, ENS = European Nuclear Society, 2013, pp. 279-284.

- Matjaž Koželj, Radko Istenič, "Radioactivity experiments for schools", In: *Proceedings*, 22nd International Conference Nuclear Energy for New Europe - NENE 2013, Bled, September 9-12, Leon Cizelj, ed., Matjaž Leskovar, ed., Mitja Uršič, ed., Ljubljana, Nuclear Society of Slovenia, 2013, pp. 1313.1-1313.9.
- 4. Tomaž Skobe, "Travelling exhibition Fusion Expo", V: *Proceedings*, 22nd International Conference Nuclear Energy for New Europe - NENE 2013, Bled, September 9-12, Leon Cizelj, ed., Matjaž Leskovar, ed., Mitja Uršič, ed., Ljubljana, Nuclear Society of Slovenia, 2013.

RADIATION PROTECTION UNIT

SVPIS

The SVPIS has been involved in ionizing-radiation measurements and radiation protection since the commissioning of the TRIGA MARK II Research reactor in 1966. The responsibility of SVPIS is the radiation control of all the activities at the Institute dealing with ionizing radiation. Our main task is the supervision of the reactor and the 17 laboratories that use sources of ionising radiation in their research work. More than one hundred different sources are used, such as sealed sources, open sources, X-ray units and the accelerator TANDETRON, all of which need regulatory control.

SVPIS is authorized by the Slovenian radiation protection administration to perform control in industrial and research institutions dealing with open or sealed radioactive sources and X-ray units. Furthermore, we are involved in radioactive waste management.

The measurements of dose rate, contamination and gamma spectrometry are performed using an accredited method (EN ISO/IEC 17025).

Personal dosimetry

The personal doses of 123 workers that regularly or occasionally deal with ionizing radiation were monitored with Thermo Luminescent Dosimeters. The maximum individual yearly dose was 0.133 mSv. This is only 0.6 % of

the regulatory limit for occupational exposure (20 mSv per year) and 13 % of the limit for the general public (1 mSv per year). Collective dose at JSI in the year 2013 was 1.03 man mSv.

Supervision of research reactor and laboratories

The controlled area of the Research reactor, the Hot Cell Facility and the Department of Environmental Sciences was monitored on a weekly basis. During some activities the constant presence of a radiation-protection worker was needed (i.e., for the opening of activated samples or radioactive-waste management). Measurements of dose rate (Figure 1), surface contamination, contamination of different objects and personal contamination were performed routinely. In most cases, no or very low contamination levels could be measured in the controlled areas.

In 2013 we performed 18 inspections in other JSI laboratories. An independent inspection by an external authorized institution was performed in the SVPIS laboratory and two additional laboratories at the JSI. There were no deficiencies recognized that could be important for radiation protection.

At present, 107 sources of radiation are used, which require regulatory control. Additionally, 384 low-activity sources are also used in different laboratories.

Environmental measurements

The environmental monitoring of the Reactor Center was performed in accordance with the existing program. The monitoring program consists of effluent measurements and measurements of samples in the environment. The activity concentrations of the gamma emitters in water samples, filters, noble gases, soil samples and sediment samples were measured periodically. About 350 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 µSv/year. The public exposure in 2013 due to activities at the Reactor Center was insignificant.

Figure 1: Dose-rate measurements near the experimental channels in the hall of the TRIGA MARK II reactor







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 radiological monitoring at Krško NPP, research reactor TRIGA and storage for low- and intermediate-level waste in Brinje.

In the field of international cooperation our staff has participated together with the Research department for low and medium energy physics (F2) and the Institute for occupational safety in the RANET exercise organised by IAEA in Japan. We performed radiological measurements (Figure 2) in the evacuated zone of the damaged Fukushima Daiichi NPP. The Slovenian team left a good impression on the proficiency level. Experience gained in the field is a good basis for future emergency planning and preparedness.

STAFF

Technical officer 1. Dr. Tinkara Bučar 2. Matjaž Stepišnik, M. Sc., Head **Technical and administrative staff** 3. Emira Bašić, B. Sc.

4. Thomas Breznik, B. Sc.

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INDEPENDENT COMPONENT PART OR A CHAPTER IN A MONOGRAPH

1. Matjaž Stepišnik, "Površinske vode", In: *Poročanje in ovrednotenje zračnih in tekočinskih imisij ter meritev zunanjega sevanja v okolici NEK*, Matjaž Korun, et al, 1. izd., Ljubljana, Institut Jožef Stefan, 2013, pp. 5-22.

SCIENTIFIC MONOGRAPH

 Matjaž Korun, Matjaž Stepišnik, Benjamin Zorko, Jasmina Kožar Logar, Gregor Omahen, Branko Vodenik, Boštjan Črnič, Katarina Vogel-Mikuš, Benjamin Zorko (urednik), Denis Glavič-Cindro (urednik), Poročanje in ovrednotenje zračnih in tekočinskih imisij ter meritev zunanjega sevanja v okolici NEK, 1. izd., Ljubljana, Institut Jožef Stefan, 2013.

CENTER FOR TECHNOLOGY TRANSFER AND INNOVATION

In January 2011 the Center for Technology Transfer and Innovation (CTT) was established at the Jozef Stefan Institute. Its principal activities are the transfer of technology and know-how from the JSI to industry as well as education and research work in the field of innovation and innovation management, and the implementation of specific technology projects.

In 2013, the Centre for Technology Transfer and Innovation (CTT) was involved in nine major projects. We have participated in EU projects from different funding-scheme programs. Within the CIP program scheme we were involved in the EEN (Enterprise Europe Network). The project EnvImpact (Increasing the impact of Central-Eastern European environment research results through more Effective dissemination and exploitation) under the 7th PF has been concluded. Under the 7th FP we continued our involvement in the TIPS (Enhancing the capacity of EU Transport Projects to transform research results into innovative products and services). Within the Alpine Space Programme we participated with the Alps4EU (Alpine Space Clusters Initiative for EU) and with the project FIDIAS (Innovative Financial Instruments for Sustainable Development and Alpine Spaces). In the context of South East Head: Europe, we participated with the project EVLIA (Making full value of good ideas by leveraging Intellectual Assets for Dr. Špela Stres financing SMEs in SEE), in the framework of the Central Europe, together with the department CT3 we continued our work on the project Central community (Emerging communities for collective innovation and Central Europe). We also work on the project IPforSMEs (The Role of Intellectual Property (IP) and creating regional value through

interregional exchange IP) under the Cross-Border Cooperation Slovenia-Italy. We were also involved in national projects: we started our activities on the project KTT (Consortium for technology transfer), ZS (Scientific meetings, ARRS) and concluded our work on the project TP PROINCOR (Technology Park Ljubljana). We also carried out some commercial projects with a small contract value.

We maintain an online entry point with a set of JSI competencies to

communicate with business partners and the general public at http://tehnologije.ijs.si. We were involved in the establishment of two spin-out companies and we were supporting researchers in the preparation of two proposals for spin-out companies. In 2013 we dealt with 10 invention disclosures and with 4 patent applications. In 2013 we conducted over 40 different cases related to the JSI's intellectual property, we established the proper legal basis and contracts in all cases where it was necessary (10 contracts of the new type).

Assistance with intellectual property protection and the licensing/commercialization of technologies is performed, firstly by the assessment of the technology and market potential. Secondly, we review the patent databases and thirdly we help researchers protect intellectual property and help them during the implementation of the invention in the economy. We evaluated 21 technologies according to the state of the art and potential market. We run market analyses and active marketing operations for the 14 best examples of technologies.

In 2013 the activities of the Consortium for Technology Transfer (KTT) began. The consortium consists of representatives of technology transfer offices from the Jožef Stefan Institute (head of KTT), the University of Ljubljana, the National Institute of Chemistry, the University of Maribor, the National Institute of Biology and the University of Primorska. The basic activity of the consortium is to provide assistance in the managing and marketing of intellectual property and assistance in the preparation of non-disclousure agreements of trade secrets, contracts for the acquisition and marketing of technologies. Within the consortium, 45 technologies were considered in 2013, of which 33 technologies were prior to the first patent application (secret know-how). Of the remaining technologies, 9 were registered at the Intellectual Property Office (SIPO), 8 technologies were filed as international patent applications (WIPO, EPO), and 1 technology has been registered at

Our center carried out the activities within the framework of eight EU projects in different programme schemes, one cross-border project Slovenia-Italy and acquired two new projects.



We organized 35 company visits at the JSI. The researchers from the JSI, together with the industrial partners, identified 49 new development projects.



In September we organized the 6th International Technology Transfer Conference and awarded two prizes for the best innovations with a total value of €2000.



Figure 2: Award ceremony for the innovation with highest commercial potential on 6th International Technology Transfer Conference

During the JSI Week of Open Doors there were more than 1000 visitors to the Institute, with an additional 41 visits being organized throughout the year, bringing more than 1200 visitors to the Institute. In total we had over 2200 visitors.



Figure 3: JSI Open doors 2013 - 23. 3. 2013



Figure 4: JSI Open doors 2013 - 23. 3. 2013

the U.S. Patent and Trademark Office (USPTO). We had 15 cases of activities regarding the establishment of the spin-out companies, and for 8 technologies active marketing operations were carried out.

To researchers we offer the following services: assistance in patenting, licensing, creation of spin-out companies, preparing and submitting patent applications, the implementation of active marketing, and search for business partners, preparation of technology offers and technology demands, preparation of non-disclosure agreements (NDAs) and the preparation of licensing agreements and other documents related to the protection of intellectual property.

To assist in the commercialization of the R&D results, the inventors, researchers and entrepreneurs from Slovenia are turning to us. To increase the active collaboration between researchers and industry we organized visits to/from more than 35 companies and researchers have identified over 49 new development projects. We helped several research departments with the submission of European project proposals.

During the JSI Open Doors event, since 2010 called the Week of Open Doors, the Institute was visited by more than 1000 people and they learned a lot about the Institute, and the structure and activities of individual laboratories. In addition, we recorded 41 other visits (more than 1200 visitors) from kindergartens, primary schools, high schools, institutions, as well as the individuals from all over Slovenia and abroad. In total, in 2013, over 2200 people visited the Institute and learned about the work of the largest research institution in Slovenia.

Colleagues at the CTT participated, as organizers or co-organizers, at six events, as well as attending conferences, training sessions and other meetings. A total of over 30 task forces and other meetings were carried out, with the aim of establishing an integrated support environment.

We would especially like to highlight the organization of the 6th International Technology Transfer Conference, held on 17 September 2013, co-joined with Innovation Day 2013, organized by the Slovenian Chamber of Commerce. The conference awarded a prize for the most innovative project. The International Commission of the representatives of venture capital awarded a prize of €2,000 for innovative ideas coming from the Jožef Stefan Institute. At the conference we also organized meetings for companies and researchers from public research organizations. In all, 22 such meetings took place.

Organization of conferences, congresses and meetings

- 1. Organization of the week of JSI Open doors, 23. 3. 2014
- Enterprise Europe Network event co-organizer: 2nd International B2B Software Days - The Big Data Challenge, Vienna, Austria, 10. 4. 2013
- Enterprise Europe Network event co-organizer: VMC Forma Tool Brokerage Event, Brno, Czech Republic, 8.–9. 10. 2013
 - Enterprise Europe Network event co-organizer: Technology Dating, Videm, Slovenia, 17. 5. 2013
 - Organization of Young researchers 2013: Academic Entrepreneurship for young researchers at JSI, 24. 5. 2013
 - Organization of 6th International Technology Transfer Conference in collaboration with Innovation day 2013 - Chamber of Commerce and Industry of Slovenia, Brdo pri Kranju, Slovenia, 17. 9. 2013
 - Co-organization of TIPS training academy event: intellectual property rights; the market potential for your R&D results; funding and financing facilities to bring your research to the market; support initiatives to find potential partners for further development of your R&D results, Prague, Czech Republic, 25.–28. 11. 2013

INTERNATIONAL PROJECTS

- Evaluation of Industrial Projects for Italian Partner Veneto Innovazione Spa Dr. Špela Stres
- 7FP ENVIMPACT; Increasing the Impact of Central-Eastern European Environment Research Results through more Effective Dissemination and Exploitation European Commission Marieta Trobec. B. Sc.
- 7FP TIPS; Enhancing the Capacity of EU Transport Projects to transform Research Results into Innovative Products and Services European Commission
- Dr. Špela Stres 4. Alps 4 EU
- European Commission Dr. Špela Stres
- IPforSMEs Intellectual Property for Small and Medium Sized Companies Government Office for Local Self-Government and Regional Policy Dr. Špela Stres
- FIDIAS Innovative Financial Instruments for Sustainable Development in Alpine Space European Commission Dr. Špela Stres
- 7. CE Central Community-Emerging Communities for Collective Innovation in Central Europe

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Monograph

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- SEE; EVLIA Making Full Value of Good Ideas by Leveraging Intellectual Assets for Financing SMEs in SEE
 Leith Tachnicel Constraints See Programme
 - Joint Technical Secretariat See Programme Dr. Špela Stres
- MED FireMed; Innovative Financial Instruments to support Energy Sector SMEs in Med Area Laist Technical Constantiat Med Programme

Joint Technical Secretariat Med Programme Dr. Špela Stres

 CIP - EACI; EASME - EIC&IRC Slovenia 1, EIC&IRC Services in Suport of Business and Innovation European Commission

Marjeta Trobec, B. Sc.

R&D GRANTS AND CONTRACTS

- 1. Technology Transfer in Public research institutions dr. Špela Stres
- IPforSMEs Intellectual property for Small and Medium sized Companies Dr. Špela Stres

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- 7. Miha Goriup, B. Sc.
- 8. Dr. Duško Odić
- 9. France Podobnik, B. Sc.
- 10. Marjeta Trobec, B. Sc.
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- 11. Lea Aissatou Kane, B. Sc.

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Mentoring

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